27TH INTERNATIONAL CONFERENCE

ON SCIENCE AND TECHNOLOGY OF SYNTHETIC ELECTRONIC MATERIALS



BOOK OF ABSTRACTS

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Conference Chairs: Marco Cremona and Ivan H. Bechtold

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CONFERENCE CHAIRS

Marco Cremona

Ivan H. Bechtold

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Preface

Dear Participants,

It is with great pleasure that we present the Book of Abstracts of the 27th International Conference on Science and Technology of Synthetic Electronic Materials (ICSM 2026).

ICSM is the longest-running international conference series dedicated to the science and technology of conducting and semiconducting organic materials. Established in 1976, at a time when highly conducting molecular crystals and conjugated polymers were emerging as new and promising classes of materials, the conference evolved alongside the field and has become one of the world's foremost forums for organic and molecular electronics.

The 27th edition of ICSM was held in Rio de Janeiro, Brazil, from July 19 to 24, 2026, bringing the conference back to Brazil for the first time since 2008. ICSM 2026 also hosted the Sixth Conference on Women in Renewable Energy and Sustainability (WiRES), further expanding the scientific program and promoting important discussions on sustainability, diversity, and the role of women in science.

A central priority of the Organizing Committee was to encourage the participation of students, early-career researchers, and women, recognizing the importance of fostering new generations of scientists and promoting greater representation and diversity within our research community.

ICSM 2026 welcomed 311 participants from 29 countries, reflecting the truly international character of the conference. Approximately 35% of the participants were women, 65% were men, and 0.3% identified with another gender category. The conference community comprised 62% established professionals and 38% students. Women accounted for 37% of the invited speakers, while early-career researchers represented 31%, demonstrating our commitment to creating a more inclusive and forward-looking scientific environment.

The success of ICSM 2026 was made possible by the enthusiastic participation of the entire community and by the outstanding quality of the scientific contributions presented throughout the week. The conference provided a stimulating forum for discussing the fundamental science, latest advances, emerging applications, and future directions of organic electronics, while also creating valuable opportunities for scientific exchange, new collaborations, and lasting professional connections.

The abstracts collected in this volume offer a representative overview of the breadth, vitality, and interdisciplinary nature of the research presented at ICSM 2026. We hope that this book will serve not only as a record of the conference, but also as a source of inspiration for future scientific developments and collaborations.

We extend our sincere gratitude to all participants, speakers, authors, sponsors, exhibitors, members of the committees, volunteers, and partners whose contributions made ICSM 2026 such a memorable and successful event.

Thank you for being part of ICSM 2026.

Marco Cremona and Ivan H. Bechtold
Chairs, ICSM 2026

Summary

A complete index of contributions, arranged by scientific topic and presentation type.

CONFERENCE ABSTRACTS · 353 contributions

01 Organic Conductors and Superconductors

PLENARY PRESENTATION (1)

Spin coupling in molecular semiconductors: from solar cells to quantum technologies 1

INVITED PRESENTATION (5)

2D π-Conjugated Polymers and Covalent Organic Frameworks: from Dirac Metals to Porous Heterojunctions 2

Conjugated polymers for magnetosensing and thermoelectrics 3

Molecular Control of 1D Polaron Delocalization Driving High Mobility in Indacenodithiophene Copolymers 4

Non-Nernstian Behavior in Organic Electrochemical Transistors 5

Organic 2D Crystals and van der Waals Heterostructures 6

ORAL PRESENTATION (9)

Confocal Raman, Photoluminescence, and Photocurrent Imaging of an Organic Solar Cell 7

Development of an advanced high vacuum cluster tool for the controlled growth of halide perovskite thin films. 8

Dual TADF and TTA emission in D-A-D molecules from green to deep red with mechanochromic properties 9

Electronic hair: transforming hair via conductive dyes into a bioelectronic interface for scalable electrophysiology 10

Glass-like non-equilibrium dynamics in heavily doped polymer conductors 12

One-Pot Synthesis of Aqueous PEDOT-Based Conductive Inks via Sequential RAFT/Oxidative Polymerization. 13

Selection rules and charge order pattern in BEDT-TTF κ-phase salts 14

Thermal and Light-Induced Stability Study of a High-Efficiency Vacuum-Deposited Small-Molecule OPV Donor 15

Thermally Activated Delayed Fluorescence Sensitized Blue Organic Light-Emitting Diodes 16

POSTER PRESENTATION (5)

Atomic Layer Deposition of Ultrathin Topological Semimetals with Thickness-Dependent Resistivity 17

Effect of addition carbon nanotubes (MWCNTs) on the microstructure, mechanical properties and wetting of nanocomposites Sn-Bi/MWCNTs solder alloys 18

Exciton Dynamics Modulation in Conjugated Terpolymers: The Role of Fluorescent Pendant Groups 20

Sensitive Piezoelectric Layer with Additives and Electrospun PVDF Nanofibers 21

Study of optical and structural properties of columnar liquid crystal films produced by drop-casting, spin- coating and blade-coating 22

02 π-Conjugated Molecules

PLENARY PRESENTATION (1)

Theory for synthetic electronic materials: from transport and thermoelectric conversion to light-emitting 23

INVITED PRESENTATION (11)

Adaptive Aromaticity and Its Application to Singlet Fission 24

Controlling spin by materials design in light-emitting applications: A computational perspective 25

Defects and Degradation in Organic Semiconductors – New Methods of Detection to Variables Influencing Degradation 26

From Spherical to Flattened Linear Structure: Exploring Minimal Units of Electron-Accepting Conjugated Hydrocarbons 27

Impurities in Arylboronic Esters Induce Persistent Afterglow 28

Innovation in Molecular & Thin Film Engineering for Stretchable & Functional Electronics 29

Organic Bulk Heterojunction Semiconductors for Photocatalysis and Solar Fuels 30

Spectroscopic proof of inversion of the lowest singlet and triplet energy states in the heptazine HzTFEX2. 31

Squaraine dyes: from chiral aggregates to single-component photodetectors 32

The influence of non-covalent contacts on stability in boron- containing donor-acceptor compounds designed to feature TADF 33

Summary

continued

Topological Molecular Carbons 34

ORAL PRESENTATION (35)

Aggregation-induced thermally activated delayed fluorescence in diindoloquinolinoacrydines 35

Ambient Direct Arylation Synthesis of Thienothiophene Based Copolymers with Mixed Alkoxy and Oligoether Side Chains 36

Amplified chiroptical properties of N-Heteropolycycles in the crystalline solid 38

Anti-Kasha fluorescence, ultra-long room-temperature phosphorescence and delayed fluorescence from a nearly flat non-symmetric polycyclic aromatic hydrocarbon 39

Bridgehead Annulated Triptycenes with Axial Chirality as Scaffolds for CISS and CPL Enhancement 40

Brominated Triryl Radical Modified with Carbazole Donor as a Chiral Luminescent Material 41

Charge transfer, polarons formation, and clustering of doped P3HT chains unveiled by first principle molecular dynamics 42

Electrochemical modulation of the elastic modulus of anorganic mixed electronic-ionic conductor 43

Energetic and Structural Origins of TTA Singlet-Formation Probability in Anthracene Upconversion Materials 45

Experimental and theoretical study of columnar liquid crystal arrangements of benzoperylene diimide 46

Gold-activated p-doping for organic semiconductors 47

Influence of host properties and molecular organisation on triplet–triplet annihilation upconversion 48

Light-responsive structural control in liquid crystals for solar energy storage and beyond 49

Mixed Micelle Thermodynamics and Interfacial Control in Surfactant-Assisted Sol–Gel Ga2O3 Thin Films 50

Modulating Singlet-Triplet Transitions in Benzofluorene Diradicals via Conformational Locking of Quinoidal/Aromatic Hybrid 51

Nanoengineered organic pi-conjugated donor-acceptor- donor trimers particles for photocatalytic H2 evolution 52

Organic Electrode Materials with Defined 3D Structures for Multivalent Metal-Ion Batteries 53

Red-emitting dimethoxy/difluorobenzothiadiazoles core materials for OLED with stable warm-white electroluminescence 54

Room temperature Coulomb gap signatures in PEDOT 55

Sequence-defined Pi-conjugated Oligomers for Organic Electronic Devices 56

Spectroscopic ellipsometry characterization of thin films for application in OPVs 57

Spectroscopy to Unravel Symmetry Breaking Structure- Property Relationships aimed at Two-Photon Absorption for Cell Imaging 58

Supramolecular control of excited-state pathways in organic emitters: from TADF and RTP to sensing and singlet oxygen generation 59

Synthesis and photophysical properties of benzoyl-peri- xanthenoxanthenes. Intensely fluorescent ketones. 60

Synthesis engineering and development of emergent conducting pi-conjugated materials: applications in energy harvesting and storage devices 61

Tetrameric Architecture of Non-fullerene Acceptors for Improved Morphology and Stable Organic Solar Cells 63

The place of iridium complexes on the phosphorescence - TADF spectrum: Evidence for thermally activated delayed fluorescence in iridium(III) complexes 65

The transition between direct and inverted singlet-triplet gaps in nitrogen-substituted phenalene molecules 66

Thickness-Dependent Molecular Orientation in Organic Layers: Insights from Single-Molecule Microscopy on Ensemble Trends 67

Tracking excited-state proton transfer in aromatic compounds 69

Tuning Optoelectronic Properties of Organic Semiconductors through Boron-Nitrogen moieties 70

Ultrafast Photoconversion Drives Fluorescence Switching in anthracene-functionalized β-diketones 71

Understanding phodecomposition and controlling the singly occupied molecular orbital of polychlorinated triarylmethyl radicals 72

Unlocking Trityl Acceptor Polyradicals 74

π-Extended N-Heterocyclic Carbenes: A Platform for Excited-State Control 75

POSTER PRESENTATION (39)

Competing copolymer and terpolymer formation in Suzuki reactions: an experimental and thermodynamic insight. 76

Conjugated Polymer-TEMPO Hybrid Electrodes for electrocatalytic Alcohol Oxidation 77

Connectivity and torsional control of TADF in Carbazole-Triazine star-shaped emitters 78

Crystalline Host–Guest Geometry Locking for High-Speed RISC in TADF Emitters 79

Design and Synthesis of Dithienothiophene-Based Donor–Acceptor Conjugated Polymers for Energy Applications 80

Diphenyl sulphone core carbazole dendrimers for blue light-emitting electrochemical cells 82

Dyads Derived from 3,5-Dimethylphenol and 1,8-Naphthalimide: Synthesis, Characterization, and Applications 83

Summary

continued

Effect of Molecular Structure on the Interfacial Organization and Rheology of Langmuir Monolayers **84**

Electronic Structure and Spin Coupling in Blatter Radical–Fused Phthalocyanines: A DFT Study **85**

From Partly Bridged Triphenylamines to Azatriangulenes **86**

Giant surface potential of vacuum-deposited carbazole dendrimers films with fluorinated substituents **87**

High-Performance Organic Mixed Ionic-Electronic Conductors Enabled by Thienoisoindigo-Based Polymers **88**

Homeotropic alignment study on a two liquid-crystal blend **89**

Influence of π-Conjugated Polymer Nanoparticles on the Photo- and Thermal Stability of Chitosan Films **90**

Insights into core-level excitations in non-fullerene acceptors **91**

Interaction Between Benzothiadiazolyl triazole Molecules and the Non-Fullerene Acceptor Y18 **92**

Investigation of solvent-driven chain packing in the bulk of P3HT using MD simulations **93**

Lignin Biomass Valorisation to High Value-Added Chemicals (phenol and benzaldehyde) using g-C3N4 nanomaterials **94**

Mechanistic Origin of Photodegradation and Impurity Effects in Donor–Acceptor Luminescent Radicals **95**

Modulating Anti-Kasha Fluorescence and Phosphorescence in Azulene Derivatives **96**

Modulation of Photoinduced Electron Transfer by Sulfur-to-Selenium Substitution in Benzazole Systems: A Fluorescence Quenching Study **97**

Molecular modeling of arylazopyrazole surfactants: photophysical and self-assembly properties **98**

Monte Carlo Modeling of Flexible Amphiphile Self-Assembly: Energetics, Chain Stiffness, and Micelle Formation **99**

Multifunctional Discotic Liquid Crystals Based on Acylhydrazones **100**

Organic and flexible colorimetric sensor for the detection of copper ions in water and Cachaça **102**

Organic Hyperbolic Materials for Optoelectronic Applications **104**

Organic π-Diradicals in Action **105**

Perylene Diimide Encapsulation with the Mechanical **106**

Photoinduced Enhancement of Fluorescence Quantum Yield in an Isoxazoline–Carbazole Derivative **107**

Quantum Yield of Perylene-Derived Emitters Improved by Crystalline Liquid Host Alignment **108**

Silicon Phthalocyanines: From Air Stable N-Type To Record Breaking P-Type Performance In OTFTs **110**

Solvent and Solid-State Effects on the Photophysical Properties of Benzothiadiazole and Benzoselenadiazole Derivatives **111**

Strategic Design of Optically Active Molecules: The Impact of Central and Peripheral Group Substitutions **112**

Substituted Trichlorotriphenylmethyl-based Radicals: Design, Synthesis and Photophysical Properties **113**

Synthesis and application of D-A-D fluorescent organic molecules in luminescent solar concentrators (LSCs), visible light communication (VLC) and photocatalysis. **114**

Synthesis and evaluation of novel D-A-D and A-D-A fluorene-based photosensitizers for DSSC **115**

Thienothiophene Based Conjugated Materials for Organic Electronics **116**

Tris(aryloxadiazolyl)triazines and Tris(aryloxadiazolyl)benzenesAnalogous stars with different mesomorphic behavior **117**

Tris(N-phenyltriazole) Liquid Crystalline Matrices for Anisotropic Emission **118**

03 Organic and Hybrid Electronics

INVITED PRESENTATION (14)

(Photo)catalytic doping of organic semiconductors **119**

Advanced photophysical analysis for elucidating excited-state energy configurations in TADF Materials **120**

Breaking linear scaling relationships in electrocatalytic nitrate reduction to ammonia with high-entropy alloys **121**

Design of thermally activated delayed fluorescence materials for high-performance solution-processed organic light-emitting diodes **122**

Generating Fuels from Sunlight Using Polymer Photoelectrodes **123**

Hybrid thin film materials for sustainable energy devices **124**

Is Polarity Intrinsic? Redefining Charge Transport in Organic Semiconductors through Interfacial Physics **125**

Nanostructured Materials for Chemical Sensing: 2D Nanomaterials and Electrospun Platforms **126**

Scale-up challenges for third-generation PV | Case comparison for Perovskite- and Organic-PV **127**

Studies of exciton loss processes in OLEDs assisted by kinetic Monte Carlo simulations **128**

Sub-microsecond Delayed Fluorescence Enabled by Molecular Engineering of Triazatruxene Emitters for High-Performance OLEDs with Suppressed Efficiency Roll-off **129**

Towards a conformable, sustainable and multifunctional organic field-effect transistor platform **131**

Vertical Organic Electrochemical Transistors and Neuromorphic Devices **132**

Summary

continued

Wafer-scale organic single crystals: integrated circuits and quantum charge transport **133**

ORAL PRESENTATION (62)

A photo-patternable solid-state electrolyte for high-performance, miniaturized, and implantable organic electrochemical transistor-based circuits **134**

Advancing the Scale-Up of Third-Generation Photovoltaic Devices: Deposition Process Stability, Repeatability, and Reproducibility **135**

Air-Processed Inverted PM6:Y6 Solar Cells on Glass/FTO **136**

An analytical model for antiambipolar organic electrochemical transistors **137**

Charge Carrier Transport and Trap Levels on Solution- Processed Zn(II) Schiff Bases OLEDs **138**

Charge Transport and Doping Physics in Mixed Lead–Tin Perovskites **140**

Comparative Study of Organic and Inorganic Electron Transport Layers for Organic Solar Cells **141**

Compositional Self-Doping in FA/Cs Perovskites for All- Perovskite Homojunction Solar Cells **142**

Contact resistance dependence on the surface-functionalization time in bottom-contact organic thin- film transistors **143**

Critical Assessment of Mobility and Contact Resistance in Metal Halide Perovskite Field-Effect Transistors **144**

Cross-linked naphthalene diimide small molecules as multifunctional electron transport layers for perovskite solar cells **145**

Design of photonic electrophoretic devices based on hybrid silica-polymer colloids **146**

Design rules to minimize the non-radiative voltage loss in organic solar cells **147**

Designing a Carbon Nanotubes/MoS_2/Prussian Blue Three-Component Nanoarchitecture for Superior Aqueous Potassium-Ion Storage **148**

Edible Organic Electrochemical Transistor for pH Sensing: Gate-Driven Mechanism and Device Physics **149**

Effect of Copper Particle Morphology on Conductive COC Composites for 3D Printing **150**

Electroluminescent photoresist enabling sub-diffraction nanopatterning of full-color OLED displays **151**

Electron Boost: Novel n-Dopants for Organic Photovoltaics **152**

Electropolymerized Polyaniline Copolymers on Carbon Fibers for Supercapacitor Applications **153**

Fabrication and temperature-dependent magnetotransport of organic spin valves using an NDI- based semiconductor active layer **154**

From Growth Conditions to Thermal Response: Reversible Polymorphism in SiPc Thin Films **155**

Furan-Based A-D-A Non-Fullerene Acceptors for Organic Photovoltaics **157**

High-performance hybrid supercapacitors based on magnesium molybdenum selenide architecture and biomass carbon **158**

High-performance Y6 homojunction organic solar cells **159**

Highly Conductive Porous MOF Thin Films Enabled by Controlled Interfacial Oxidation **160**

Hybrids of Conducting Polymers and Graphene Derivatives for Electrochemical Sensor Applications **161**

Improved performance of PM6:Y6-based organic solar cells by introducing a layer of metallic nanoparticles into its structure. **163**

Improving charge extraction in organic photoanodes via n-type SAM modification of buried ZnO/organic interfaces **164**

Interface Regulation of Oxygen Evolution Cocatalysts towards Efficient Solar-Driven Water Splitting **165**

Interfacial Siloxane Interactions to Enhance Semiconductor Ordering and Performance in Organic Thin-Film Transistors. **166**

Investigating Structure-Property Relationships of Poly(Ionic Liquids) for Gating Materials in Organic Thin-Film Transistors **168**

Kinetic Monte Carlo modelling of organic optoelectronic devices for optical communication **170**

Large scale determination of frontier orbital energies in small molecule organic semiconductors via exciplexes **171**

Mapping Electric-Fields within Polymeric Field-Effect Transistors by Sum-Frequency Microscopy **172**

Materials Acceleration Platforms: toward the laboratory of the future for perovskite and organic PV research **173**

Microstructural Studies of Solution-Processed Organic Optoelectronic Materials **174**

Modeling steady-state responses of organic electrochemical transistors based on drift-diffusion fundamentals **175**

Molecular Weight Engineering of PSS for Enhanced Thermoelectric Properties in PEDOT:PSS **176**

Multiscale Interface Engineering in Conjugated Polymers and Hybrid Perovskites **177**

Narrowband absorbing aggregates of merocyanine dyes in solution and solid state **178**

Organic complementary inverters based on inverted coplanar thin-film transistors employing different contact functionalization **179**

Persistent radicals in for pattern recognition of electrical and multicolor optical stimuli **180**

Processing-structure-property relationship in fully solution processed multilayer P(VDF-TrFE) piezoelectrics **181**

Skew-Gaussian Device Design and Application for Realistic Gaussian Distribution Representation **182**

Summary

continued

Surfactant-free organic nanoparticle dispersions for light-harvesting applications **183**

Temperature-dependent structural fluctuations govern charge transport in hybrid tin-halide perovskites thin film transistors **184**

Template Quality Dependent Conversion Synthesis of Boron Nitride Coated Graphene Hybrid Aerogels for Ultrasensitive and Selective Ammonia Sensing **186**

Terminal group effects on SAMs packing and perovskite interfacial energetics **187**

Thermal potential induced redox reaction enabled ionic thermoelectric generator **189**

Thermoelectric Properties of Thiophene-Based N-type Copolymers in Doped Oriented Thin Films **190**

Thermogalvanic Cells Towards Large-scale Applications **191**

Tin perovskite quasi-2D thin films transistors: devices and low temperature charge transport study **192**

Triplet loss processes in phosphorescent OLEDs: an integrated study **194**

Tunable stability and performance of fused thienothiophene based polymers for organic electrochemical transistors and artificial synapse based on a side chain reorganization strategy **195**

Understanding the impact of structural defects in conjugated polymers across various device types **196**

Understanding the underlying processes behind high performing organic homojunction solar cells **197**

Unraveling electronic structure from 2D to 2D/3D perovskite interfaces by UV-vis, electron and photoelectron spectroscopy **198**

Unveiling degradation differences of perovskite PV: from cells to modules. **199**

UVA sensor based on conducting polymer **200**

Wavelength-Selective Negative Photoconductance in ZnON phototransistor for Neuromorphic Vision **201**

ZnO thin films deposited by PE-PLD for gas sensing applications **202**

π–d Conjugated Coordination Polymers for Thermoelectric and Solar Energy Applications **203**

POSTER PRESENTATION (37)

A Dilute-Heterojunction Strategy for Probing Charge Generation in Organic Photovoltaics **205**

Composition-dependent modulation of electrical transport in WO3/CuWO4 heterostructures induced by quinoline derivative incorporation **206**

Development and Characterization of MoS_2/PEDOT:PSS Thin Films with Potential Application in VOC Sensors **207**

Dielectric Characterization of Electrospun PVDF-based Nanocomposites with Graphene Nanoplatelets **208**

Effect of deposition technique on the polyaniline-based thin films for PTMs detection **210**

Fabrication of an Amplifier Circuit Using Liquid Crystalline Organic Semiconductor Thin Film Transistors **212**

Fluorene-Decorated Donor–Acceptor Emitters with TADF and High Hole Mobility for Solid-State Picric-Acid Sensing and Sky-Blue OLEDs **213**

Gas Sensing Properties of Polythiophenes and Fullerene Derivatives **214**

Grain-Boundary-Driven Stochastic Oxide Junction in 2D SnSe Enables Dual Electrical-Optical PUFs **215**

Green Synthesis of 2D Conjugated Polymer Networks via Metal-Free Click Chemistry for High-Performance OECTs **216**

Hybrid GO-AuNPs-Silsesquioxane Nanocomposites: Synthesis, Characterization, and Electrochemical DNA Biosensing **217**

Impact of the process conditions for the deposition of the source and drain contacts on the contact resistance in organic thin-film transistors **218**

Industrial Upscaling of Organic Photovoltaic Devices: Analyzing the Transition from Stepwise Regime to Large-Area Continuous R2R Processing **219**

Inkjet-printed graphene-based electrodes for flexible organic devices on biodegradable substrates **220**

Kinetic Monte Carlo modelling of organic optoelectronic devices for optical communication **221**

Material- and System-Level Characterization of Metal Alloy Thin Films for Near-Field Magnetic EMI Suppression in Smart Electronics **222**

Materials for Quantum Information Science **223**

Mechanistic modelling of exciton-polaron quenching in thermally activated delayed fluorescence emitters **224**

Memristive self-assembled multilayers of octahedral ruthenium complexes with non-innocent redox-active ligands **225**

Multi-heterojunctioned plastics with high thermoelectric figure of merit **226**

Nanostructured Films and Nanofibers Using Low-Bandgap Polymer-Based Sensitive Surfaces to Detect **227**

Nanostructured Polyaniline Films Prepared by the Langmuir-Schaefer Technique for the Development of Sensing Platforms **229**

Near-/Far-Field Evaluation of Conducting–Magnetic Thin Films for Radiated-EM Energy Mitigation in Smart Hybrid Electronics **230**

On the importance of reduced interpenetration of donor-acceptor interfaces in light harvesting capacitors: a comparison of small molecule vs. polymeric acceptor materials **231**

One-Pot Synthesis of Nanoarchitectured Thin Films Formed by Carbon Nanomaterials and Metal Nanoparticles Deposited on Silica Substrate for Optical Applications **232**

Performance Optimization of Environmental Sensors: Investigating Non-Fullerene Thin-Films for Enhanced Humidity Detection **234**

Summary

continued

Performance Optimization of OFETs by Interface Functionalization with loosely packed Self-Assembled Monolayers 236

Probing charge extraction and recombination in fullerene and non-fullerene photovoltaic by transient optical and electrical measurements 237

Scalability of water-based nanoparticles for active layers in organic photovoltaics 238

Screen-Gate Based Organic Transistors for Adaptive Sigmoid and Gaussian Activation Functions 240

Solid Dopant Matrices Based on Microfibrillated Cellulose and KCl for High Performance Organic Transistors 241

Surface Thermodynamics, Wettability, and Optoelectronic Properties of Anodized Al_2O_3 Films Under Programmable Voltage Control 243

Thermal Cycling-Driven Degradation of Perovskite Solar Cells by In Operando nano-XRD 245

Tuning the Operating Mode of P3HT Electrolyte-Gated Transistors by Controlling Extra Ions Mixed into a Honey-Based Electrolyte 246

Urbach Energy in MEH-PPV 247

Urban deployment and performance analysis of organic photovoltaic devices: Experimental and theoretical insights 249

Water-based nanoparticle-printed thin films for scalable and sustainable organic photovoltaic devices 251

04 Organic and Hybrid Photonics

PLENARY PRESENTATION (2)

Cool plastics for a greener world 252

The rise of organic and inorganic two-dimensional materials for interface engineering in perovskite photovoltaics 253

INVITED PRESENTATION (18)

Chiral Optoelectronics for Next-Generation Displays and Photodetectors 254

Chiroptical switching and logic operations using photoexcited states 255

Connecting Mechanical Properties, Durability, and Reliability of Perovskite Solar Cells 256

Contact Modulation in Perovskite/Organic Optoelectronic Device 257

Design and Synthesis of Functional Organic Materials for Hybrid Photonic Devices 258

From Displays to Data Links: High-Speed Organic Optoelectronics for Visible Light Communication 259

Hybrid Perovskite Photodetectors 260

Integrated Energy Harvesting and Storage for Autonomous Sensor Networks 261

Interface engineering for improved efficiency and lifetime in organic solar-cells 262

Narrow OLED Emitters by Multiresonant Dyes based on Aromatic/Antiaromatic and Quinoidal Designs 263

Organic semiconductors as a platform for molecular photonics: from polariton devices to fluid light and neural interfaces 264

Photo- and Thermal-Stability of Organic Solar Cells 265

Photokineticism: Comprehensive and quantitative understanding of phenomena from elementary processes 266

Towards scalable fabrication of Sn and Sn/Pb perovskites solar cells 267

Twisting Light and Spin in Chiral Halide Perovskites 268

Understanding the Role of Molecular Structure, Conformation and Spin Orbit Coupling in Intersystem Crossing of TADF Emitters 269

Vapor phase deposited perovskites; how to improve the photoluminescence quantum yield? 270

Wearable organic optoelectronics for display and healthcare applications 271

ORAL PRESENTATION (34)

Active conducting polymer metaoptics 272

Anti-Kasha Emission in Difluorenothiophene Diradicals: Impact of Donor-Acceptor Substitution 273

CdSe Quantum Dots for Interface Passivation in Perovskite Solar Cells 274

Coinage Metal TADF Emitters for Stable OLEDs and Nonlinear Photonics 275

Control of the photoluminescence quantum yield of noble metal organometallic nanocomposites by pulsed laser driven CO2 reduction reaction 276

Controlling Nanoscale Interfacial Reorganization to Extend Electrochemiluminescent Device Lifetime 277

Degradation study of red hyperfluorescent OLED devices based on TXO-TPA and DBP as TADF assistant and fluorescent emitter respectively 278

Donor-dependent photophysical pathways in Organic bulk heterojunction solar cells 279

Electrochromic Smart Windows: Achieving an Absolute Private State through Thermochromically Engineered Electrolyte 280

Engineering Delayed Emission in Phenanthrene Diketal Emitters for OLEDs 281

Evaluation of Molecular alignment, Mobility, and Photodiode Characteristics in Liquid Crystalline Organic Semiconductor Bulk Heterojunction Films 282

From Interface to Bulk: Hierarchical Integration of Quantum Dots in Perovskite Solar Cells 283

Herzberg–Teller Effect as a Phonon-Assisted Optical Transition 285

High-Mobility, Short-Lifetime Organic Emitters Enabling High-Speed Modulation in OLEDs for Visible Light Communication 286

Summary

continued

How Multiple RISC Pathways Shape Efficiency and Roll- off in TADF OLEDs **288**

Light-Induced True Random Number Generation in Bipolar Photo-Responsive Devices for Hardware Deepfake Security **289**

Materials to enable new-generation photovoltaics at industrial scale **290**

Mobility imbalance as a design paradigm for ultrafast organic photodetectors in optical communication **291**

Modeling Environmental Effects on the Electronic Properties of Bulk Heterojunctions for Organic Solar Cells **292**

Nanostructures for efficient organic light-emitting diode emission management **293**

Organic electronicsbased on thienothiophene and ditihienothiophene **294**

Protonation-Mediated Delayed Emission in Organic Materials: Dynamic Control of Triplet Excitons via Hydrogen-Bonded Environments **295**

Pushing the boundaries of the energy gap law: Near-infrared TADF material spectroscopy **297**

Reducing singlet-triplet annihilation losses in hyperfluorescent OLEDS and organic lasers **298**

Revealing and eliminating surface-localized defects for high-performance ambient-processed organic optoelectronics **299**

Simulating TTM-Based Diradicals: Bridge, Substituent and Vibronic Effects on Excited-State Dynamics **300**

Skin-Conformal MHz-Speed Organic Photodetectors for Long-Range Near-Infrared Communication **301**

The Many Roles of Host Materials in Single-Layer Blue OLEDs: Enabling Ohmic Charge Injection, Balanced Transport, and Enhanced Stability **302**

Thermally activated delayed fluorescence (TADF) in indolizine derivatives: excited-state photophysics under photoexcitation and electroexcitation. **303**

Towards continuous wave organic lasing: A triplet–triplet annihilation upconversion approach to triplet management. **305**

Ultrafast Structural Dynamics in Luminescence Process in Crystalline Carbazole Benzonitrile Derivatives **306**

Understanding the photophysical origin of efficiency roll-off in TADF OLEDs **307**

Vacuum-processed organic and perovskite optoelectronics: challenges and opportunities in architecture and device engineering **308**

Zinc Tin Oxide Nanocomposite Deep UV Photodetector Embedded Circuit for Wireless Flame Detection **309**

POSTER PRESENTATION (22)

A Pyridine-3,5-dicarbonitrile Emitter with Polymorphism-Dependent Luminescence and Efficient OLED Performance **310**

Correlated 1/f³ Noise in Photo-NDR DNTT/TiO2 Heterojunctions for Secure Bio-signal **311**

Delocalisation enables efficient inter-chain exciton separation in conjugated polymers **312**

Development of a TiO2-Nb- Based anodic Electrode for Enhanced Photovoltaic Conversion Efficiency in DSSCs **313**

Dual-Chromophore Isolation Strategies for Efficient Upconversion in TADF Emitters via Rigid, Covalent Bridges **315**

Effect of composition on thermally evaporated $CsPbBr_3$–Cs_4PbBr_6 thin films to promote radiative recombination in efficient and stable optoelectronic devices **316**

Environmental Stability of Carbazole-based Self-Assembled Monolayers in Organic Solar Cells under the ISOS-O-2 Outdoor protocol **318**

From Molecular Structure to Device Stability: BDT and BODIPY-Based Materials for OPV and OLED Applications **319**

From Solution to Device: Aggregation-Induced Enhanced Emission and twisted intramolecular charge transfer in a Pyridylcarbodinitrile for tunable Photoluminescence and OLED applications **321**

Functional Organic Materials for Sustainable Photonics: Room-Temperature Phosphorescence - Matrix Effects Tunnelling Phosphorescence Lifetime **323**

Heteroleptic Copper(I) and Silver(I) Complexes for Light-Emitting Devices **325**

Higher-Order Harmonics Probed by Nonlinear Impedance Spectroscopy in Perovskite Solar Cells Based on Niobium MXenes **326**

Hole Trap Formation in Quantum Dot Light-Emitting Diodes Under Electrical Stress **327**

HS- OLEDs using indolocarbazole-based emitters with balanced charge transport and enhanced solid-state emission **328**

Hyperfluorescent Host-Free OLEDs for Organic Upconversion Devices **329**

Interfacial Modulation in Hybrid Emitters Based on Rare-Earth Doped TiO2 and D-π-A Quinoline Derivatives **331**

Ion Migration and Hysteresis in Perovskite Solar Cells: Insights from Capacitance-Frequency Analysis **332**

Nanostructures for efficient organic light-emitting diode emission management **333**

Phosphorescent Exciplexes **334**

Preliminary Photophysical Investigation of a Naturally Derived Luminophore: Green Extraction, Aggregation Dynamics, and Enhanced Room-Temperature Phosphorescence in Poly(acrylic acid) Matrix. **335**

Spatially resolved phonon lifetime evolution under pulsed laser perturbation in radiation-damaged crystalline systems **337**

Summary

continued

Study of γ-butyrolactone (GBL) as solvent for recycling Perovskite Solar Cells (PSCs) 338

05 Bioinspired Materials, Devices and Applications

PLENARY PRESENTATION (1)

Commercializing Conformal Soft Electronics for Healthcare and Aged Care 340

INVITED PRESENTATION (12)

Biomimetic Electronic Polymers for Tissue-Interfaced Continuous Biosensing 341
Biorecognition across lengthscales with electrolyte gated organic transistors 342
Conducting polymer devices for hosting and monitoring in vitro models of the gut 343
Light harvesϴng with organic molecular materials: insights from ϴme-resolved spectroscopic studies 344
Organic Retinomorphic Imager and Electrochemical Transistor for Environmental Monitoring 345
Performance Enhancement in Mixed Ionic-Electronic Conductors by Molecular Design, Blend and Architecture Engineering 346
Plasmonic Nanomaterials as Dual-Action Agents for Light-Triggered Cancer Therapy 347
Polymer nanoparticles optically control the cell fate 348
Polymeric Mixed Conductors for Bioelectronic Sensors 349
Resorbable organic semiconductor devices for post-surgical monitoring 350
The Road to “Green” in Organic Bioelectronics 351
Wireless Piezoelectric Stimulation of Cells via Ultrasound-Responsive Polymeric Nanomaterials 352

ORAL PRESENTATION (14)

A Nanotube-Confined Tellurium Neuromorphic Visual System for Image Processing and Reservoir Computing 353
A Versatile, Biomimetic, 3D Electrochemical Device for Monitoring Cell Growth and Epithelial Barrier Integrity 355
Bioinspired redox membranes for stable, high-charge- injection organic electrodes 356
Dissipative Charge Transport and Electrochemical Strain Waves in Organic Mixed Ionic-Electronic Conductors for Bioelectronics 358
Excited State Opto-Ionic Reservoir Computing in Hybrid Perovskite Electrochemically-Gated Luminescent Cells 359
Interfacial Mechanics of Acetogenins in Tumor Membrane Models: the Impact of Chain Unsaturation 360
Langmuir–Blodgett Thin-Film Immobilization of Urease Hybrid Nanoflowers for Capacitive Urea Biosensing 361
Near-Infrared Phototherapeutic Nanoplatforms Based on Gold Shell-Isolated Nanoparticles for Targeting Cancer Cells 363
Recalibration-Free Multi-Day Wearable Electrophysiology Using Carbon Nanotube Dry Electrodes 365
Reservoir Computing using Organic Mixed Ionic Electronic Conductors 366
Single-Transistor Organic Electrochemical Neurons for Dense, Flexible, and Bio-Realistic Neuromorphic Systems 367
Supramolecular Hybrid Hydrogels from Cellulose Nanofibrils and Fmoc-Diphenylalanine for Biomedical Applications 368
The impact of dynamic disorder on transport in doped semiconducting polymers 369
Water soluble emissive diradicals for quantum biosensing 370

POSTER PRESENTATION (20)

3D-Printed Hollow Carbon-Paste Microneedle Electrodes as Electroactive Platforms for Future Immunosensing Applications 371
Beer-Gated ZnO Transistors for Contamination Detection 372
Development of active packaging using a ternary blend of Poly(butylene adipate co-terephthalate), poly(lactic acid), and thermoplastic starch 374
Effects of Different Concentrations Gadolinium and Yttrium doping on the Structural and Vibrational Properties of Molybdenum Trioxide with Potential application for Gas Sensing 375
Electrochemical detection of heavy metals using hybrid conjugated polymer/silver nanoparticle-based electrodes 377
Electropolymerized poly(p-phenylenediamine) films for electrochemical detection of DNA nucleobases 378
Eumelanin pigment-based doping for thermopower improvement in PEDOT:PSS blends 380
Exploiting capacitive effects within a Saxitoxin aptamer-based biosensor 381
Halogen-Terminated Ti_3C_2 MXenes for Interface Engineering in Perovskite Solar Cells 382
Hybrid PCL membranes incorporating Au and Pt nanoparticles produced by PLAL for tunable angiogenesis control 384
Influence of mucins on the membrane interaction of conjugated nanopolymer 386
Laser Induced Periodic Surface Structures on Eutectic Gallium-Indium Based Composites for Tissue Engineering 388

Summary

continued

Light-Responsive Conjugated Polymer Thin Films: Optical Sensing and an Attract-and-Eliminate Strategy for Biomphalaria 389

Methylene Violet 3RAX for Photodynamic Therapy of Melanoma 391

Near-infrared activated gold nanostars for efficient photothermal therapy of colorectal cancer 392

Neuromorphic behavior in thin films of polythiophene derivatives 393

Strain-modulated flexible bio-organic/graphene/pet sensors based on dna-curcumin biopolymer 395

Synergistic NIR-Activated Phototherapy Mediated by Gold Shell-Isolated Nanostars Conjugated to ICG 396

Targeted Photodynamic–Photothermal Nanoplatform for Improved Melanoma Treatment 397

Ultrasensitive microRNA Biosensing Through Reduced Graphene Oxide Electrolyte Gated Transistors with Machine Learning 398

06 Women in Renewable Energy and Sustainability

INVITED PRESENTATION (7)

Electronic Structure of Halide Perovskite Materials for Energy Conversion Applications 399

Generating Charges in Organic Photovoltaic Systems 400

Light as a tool in Energy and environment. Perspectives and discussions 401

Navigating the dopant:host phase space to rationalize chemical doping of semiconducting polymers: A journey from excitons, polarons to trions 402

Rational Design and Operando Understanding of Catalytic Sites for Renewable Energy and Sustainable Carbon Conversion 403

Showcasing multitasking: multiparametric biosensing examples using PEDOT:PSS devices 404

Sn/Pb perovskites challenges and opportunities for photovoltaics 405

POSTER PRESENTATION (3)

Gate-Driven Edible OECTs for Sustainable and Low-Power Gastrointestinal pH Sensing 406

Photoelectrocatalytic Study of Electrodeposited Nickel Oxide Films for Glycerol Oxidation 407

Use of metal alloys to reduce instability in perovskite solar cells 408

ROUND TABLE (1)

WiRES Round Table Discussion 409

Spin coupling in molecular semiconductors: from solar cells to quantum technologies

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Polyaromatic molecules play a key role in next-generation energy devices, with applications ranging from energy-harvesting in e.g. flexible solar cells, to low-energy operation in e.g. organic light emitting devices and unconventional computing. The photophysical properties of the materials also enable unique generation and utilisation of electronic spins, which are attractive in quantum applications, including communication and sensing.

This presentation will consider archetypal small molecule semiconductor thin films deposited using vacuum-based techniques, and focus on the structure-property relationship of spin-based properties. The crystal orientation of the films will be tailored at the macro and nanoscale, providing a platform to elucidate key anisotropic quantities such as magnetic coupling, charge transport and spin lifetime. Molecules that contain a ground state electronic spin will be contrasted with diamagnetic systems where the spin is obtained through photoexcitation, as is the case for pentacene. Applications considered firstly involve singlet fission, which can boost the performance of solar cells by generating two charges for every photon absorbed in neighbouring pentacene molecules. The mechanism of fission is interpreted via molecular film design, electron spin resonance spectroscopy, and temperature-dependent spectroscopy, with perspectives for utilising the initial state of fission in quantum information and computing [1,2]. In isolated pentacene molecules, the spin-polarised triplet states can be harnessed in a range of applications, and pentacene films exhibit competitive sensitivities in quantum-enhanced magnetic field detection [3].

[1] D. V. Lubert-Perquel et al. *Nat. Commun*. **9** (2018) 4222.

[2] K. E. Smyser and J. D. Eaves, *Sci. Rep*. **10** (2020) 18480.

[3] S. K. Mann et al. *J. Amer Chem. Soc.* **147** (2025) 22911.

2D π-Conjugated Polymers and Covalent Organic Frameworks: from Dirac Metals to Porous Heterojunctions

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Delocalized electronic states in graphene and other 2D inorganic materials give rise to various quantum phenomena that underpin their unique electronic and magnetic properties. In principle, some of these properties could be harvested in organic 2D π-conjugated polymers. In practice, the observed charge-transport behavior in such materials is controlled by the defects, and, despite the enormous recent efforts, they generally remain inferior to the best 1D conjugated polymers. In this presentation, I will focus on our recent work on understanding electronic doping in 2D polymers, including individual monolayers[1] and stacked multilayer materials[2], a.k.a. covalent organic frameworks (COFs). I will discuss our approaches to improving electron conjugation in 2D COFs[3] and, time permitting, share our most recent results on the design of COF heterojunctions for CO2 photoreduction.

[1] D. Dettmann et al. *under review* (10.26434/chemrxiv-2025-vrlkc)
[2] C.-W. Kang et al. *JACS* **2025**, *147*, 36320.
[3] Z. He et al. *JACS* **2026**, 10.1021/jacs.5c20548.

Conjugated polymers for magnetosensing and thermoelectrics

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Keywords: conjugated polymers; organic magnetoresistance; bipolarons; thermoelectrics;

Conjugated polymer semiconductors, mainly comprising light elements such as hydrogen and carbon, have intriguing spin-related properties. In particular, even in the absence of injecting ferromagnetic electrodes, a sizeable intrinsic magnetoresistance (MR) could be measured mainly in organic diodes. In this talk, I will present a mechanistic understanding of such phenomenon that puts together experimental (low-temperature electrical characterization in field-effect transistors, structural, spectroscopic and morphological characterization) and a solid computational/theoretical analysis. Such a combined approach allows to establish a relationship between polymer structure and its ability to display magnetoresistance. An additional picture on bipolaron formation at the dielectric/semiconductor and metal/semiconductor will be given.
My talk will also cover some novel polymer structures and their use for thermoelectric applications.

Molecular Control of 1D Polaron Delocalization Driving High Mobility in Indacenodithiophene Copolymers

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Keywords: Organic Field Effect Transistors, 1D conductors, IDT

Indacenodithiophene (IDT)-based conjugated polymers have been attracting much interest for having good charge mobility despite lacking long range order. Poly(indacenodithiophene-co-benzothiadiazole) (p(IDT-BT), which serves as a benchmark, exhibits remarkably low energetic disorder and high hole mobility even in a near-amorphous microstructure. This high performance is traced to its planar backbone, which fosters substantial intrachain polaron delocalization. Macroscopic charge transport is completed by sparse but efficient interchain contacts between acceptor units, effectively "stitching" the material together.[1] A reduction in backbone planarity, as seen in poly(indacenodithiophene-co-benzopyrollodione) (p(IDT-BPD)), has a dramatic effect, increasing static energetic disorder and reducing monomer-to-monomer electronic coupling. This disruption forces charge carriers to become severely localized onto single IDT donor units. This result confirms that intrachain delocalization and efficient interchain coupling are paramount providing a generalized structural design principle for high-performance pi-conjugated semiconductors.

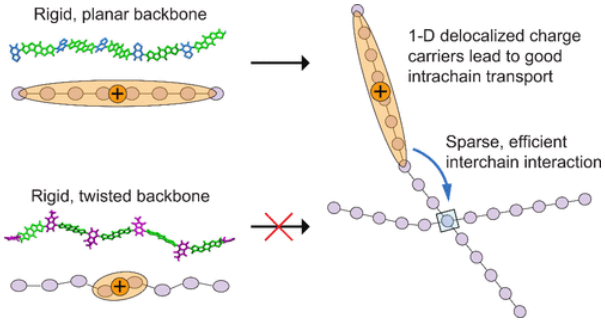


Figure 1: Illustration of charge delocalization in IDT-based copolymers

References:

[1] G. LeCroy, R. Ghosh, P. Sommerville, C. Burke, H. Makki, K. Rozylowicz, C. Cheng, M. Weber, W. Khelifi, N. Stingelin, A. Troisi, C. Luscombe, F. C. Spano, and A. Salleo *J. Am. Chem. Soc.,* **146**, 21778 (2024).

Non-Nernstian Behavior in Organic Electrochemical Transistors

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Keywords: Electrochemical devices, Organic electrochemical transistor, Output modeling

Despite the remarkable progress achieved in organic electrochemical devices (OEDs), the fundamental processes governing their operation and sensing capabilities - especially those associated with ion-to-electron transduction—remain insufficiently understood. In particular, robust fundamental models capable of describing both the steady-state and transient behavior of OEDs, while explicitly connecting the physical chemistry of the polymer–electrolyte pair to device performance, are still lacking. Here, we provide new insights into a thermodynamics-based model that qualitatively and quantitatively describes OED operation, with particular emphasis on the organic electrochemical transistor (OECT)[1]. Within this framework, we introduce new interpretations of conventional drain current models grounded in thermodynamic and electrochemical principles. The fitting parameters of the model are correlated with the physical and chemical properties of the polymer–electrolyte pair, and the model successfully captures trends observed in experimental data reported in the literature. Furthermore, our results indicate that non-Nernstian electrochemical behavior plays a dominant role in OECT operation. By analyzing experimental datasets, we also establish guidelines for materials selection and device design toward highly sensitive electrochemical biosensors and related OED technologies.

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References:

[1] Feitosa, B., *Mater. Horiz.*,**11**, 6007 (2024)

Organic 2D Crystals and van der Waals Heterostructures

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In the first part of this talk, I will present our recent advances in the bottom-up synthesis of highly crystalline 2D polymer crystals, particularly through on-water surface polymerization strategies. The confined water surface enables controlled 2D growth, leading to single- and few-layer 2D polymer crystals with long-range in-plane order and well-defined lattice structures. These materials exhibit extended 2D π-conjugation, tunable band structures, and high intrinsic charge-carrier mobilities. Beyond electronic transport, their ordered porous architectures also enable ion transport and interfacial electrochemical functionality, establishing organic 2D crystals as a versatile platform for electronics, optoelectronics, and energy-related applications. In the second part, I will focus on our recent realization of organic 2D van der Waals heterostructures. Using sequential on-water surface assembly, we achieve programmable layer-by-layer stacking of chemically distinct 2D polymers with defined lattice registry, stacking sequence, and thickness. This strategy enables both lattice-matched and controlled lattice-mismatched heterostructures, allowing systematic tuning of interlayer coupling. We will reveal emergent interfacial phenomena—including built-in electric fields, efficient charge separation, and diode-like rectification—that are governed by lattice matching and interfacial dipole alignment. These results establish O2DCs and their van der Waals heterostructures as a chemically programmable platform for exploring interlayer-coupled electronic, ionic, and quantum phenomena, opening new directions for functional organic electronics and beyond.

Confocal Raman, Photoluminescence, and Photocurrent Imaging of an Organic Solar Cell

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Organic solar cells (OSCs) offer a lightweight, flexible alternative to silicon photovoltaics, with advantages such as low environmental impact and high mechanical conformability. However, their lower efficiency and stability remain key challenges, requiring advanced characterization techniques to guide material and device optimisation.

Raman spectroscopy provides exceptional chemical specificity and is routinely used to obtain information about the various power efficiency-influencing properties of silicon, cadmium telluride, perovskite, III-V semiconductor, quantum dot, and organic cells. Combined with confocal microscopy, Raman spectroscopy enables micron-resolution imaging of material properties across a cell. Additionally, Raman microscopes can be configured for photoluminescence (PL) imaging; an industry standard for photovoltaic quality control. By further integrating a photocurrent imaging upgrade with the Confocal Raman Microscope, we can directly correlate Raman, PL and cell performance across a device.

This presentation will demonstrate Raman, PL, and photocurrent imaging of the same area on an OSC using an Edinburgh Instruments RM5 Confocal Raman Microscope. This correlative spectral and photocurrent imaging methodology is a powerful tool in the photovoltaic industry because it allows for an enhanced understanding of the properties of solar cells, their defects and degradation over time.

References

E. K. Solak et al., RSC Adv., 2023, 13, 12244-12269.

P. K. Nayak et al., Nat. Rev. Mater., 2019, 4, 269-285.

Q. Guo et al., Mater. Chem. Front., 2021, 5, 3257-3280.

Development of an advanced high vacuum cluster tool for the controlled growth of halide perovskite thin films.

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Vinci Technologies is developing an advanced high-vacuum deposition cluster for the thermal evaporation of metal-halide perovskites (MHP) in collaboration with partners from the research field. The cluster enables complete fabrication of MHP layers and associated materials without breaking vacuum, ensuring controlled growth conditions. The system integrates two dedicated deposition chambers for MHP layers and with a third chamber for complementary materials, all interconnected within a cluster architecture that preserves vacuum integrity throughout the process flow. A key challenge arises from the evaporation of highly volatile organic precursor, most prominently methylammonium iodide (MAI), which exhibit extremely high vapor pressures under vacuum at moderate temperatures and, in contrast to most conventional evaporated materials, vaporize isotropically. This can lead to undesired contamination of chamber walls, subsequent re-evaporation and cross-contamination between processes. One mitigation strategy relies on cryogenic shrouds within the deposition chamber, inspired by the principles of molecular beam epitaxy that were previously explored by Vinci Technologies. By condensing excess molecules on cold surfaces, this approach stabilizes deposition conditions, reduces contamination, and improves interface quality [1]. In addition, the system includes several design features to improve growth control and protect the vacuum system from corrosive organo-halide vapors. Vinci Technologies is also developing a cluster tool composed of a central transfer chamber surrounded by six process chambers. In addition to the chambers devoted to MHP processing, the cluster also integrates a sputtering chamber and an ALD chamber. The scientific interest lies in developing ITO and alumina encapsution layers for their integration into tandem solar cells [2] [3].

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Vinci Technologies

References

Ana M. Igual-Muñoz, Chemistry of Materials, 32, 19, (2020)

Roja Singh, Solar Energy Materials and Solar Cells, 205, 110289, (2020)

Wenlong Ji, Chemistry of Materials, 32, 164366, (2025)

Dual TADF and TTA emission in D-A-D molecules from green to deep red with mechanochromic properties

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Materials which display thermally activated delayed fluorescence (TADF) have been widely employed in organic light emitting diode (OLED) applications. This is because of their ability to harvest light from the triplet state, T1 allowing devices to have theoretical internal quantum efficiencies (IQEs) of 100%. Donor-acceptor-donor (D-A-D) molecules have been shown to be good candidates for TADF and efficient OLEDs [1,2]. However, obtaining efficient deep-red emitters remains a challenge due to the energy gap law as non-radiative decay is enhanced [3]. Triplet-triplet annihilation (TTA) is another mechanism of triplet harvesting, used in optoelectronic device applications, by formation of an excited singlet state from two triplet states. Here, we report two efficient regioisomeric D-A-D emitters, comprising 3,6-di-tert-butyl-9H-carbazole as both donor units and a dibenzo[a,c]phenazine-based acceptor. The molecules differ in donor substitution position, yielding T-shaped (PC8) and Y-shaped (PC16) geometries. Time-resolved photoluminescence measurements demonstrate delayed fluorescence (DF) in solution and solid state. Laser power and temperature dependence studies confirm that DF arises from a combination of TADF and TTA. In dilute films, both mechanisms contribute, while in neat films TTA dominates. Notably, PC8 neat films exhibit deep-red emission with only a moderate PLQY reduction compared to dilute films, highlighting its resistance to aggregation-induced quenching. OLED devices were fabricated with PC8 and PC16 as the active emissive layer in neat and CBP host conditions, giving electroluminescence covering green to deep-red. PC8 additionally displays mechanochromic properties. Upon exposure to different external stimuli (grinding, DCM vapour and recrystallisation), the emission colour can be reversibly switched, with PL maxima spanning 597-637 nm. This study allows the exploration of the difference in luminescent properties arising from different positioning

References

S. Brebels et al. ACS Applied Optical Materials, 3, 2583-2594 (2025)

T. Fan et al. Chemical Engineering Journal, 525, 170368 (2025)

X. Zheng et al. J. Mater. Chem. C, 3, 6970-6978 (2015)

Electronic hair: transforming hair via conductive dyes into a bioelectronic interface for scalable electrophysiology

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Hair remains a fundamental barrier to scalable and precise noninvasive electrophysiology, particularly in electroencephalography (EEG), by increasing electrode–skin impedance, degrading signal quality, and necessitating gels or rigid electrode architectures. Here, we introduce electronic hair (eHAIR), a new bioelectronic interface that transforms native hair into a conductive, ion–electron coupled sensing and amplification system.We develop two complementary conductive dye (eDYE) strategies. The first (eDYEC) applies rapid polydopamine functionalization followed by deposition of a PEDOT:PSS–dopamine composite, forming highly conductive, washable coatings suitable for temporary recordings. The second (eDYEP) is based on in situ enzymatic polymerization of PEDOT-based conductors directly on individual hair strands, providing semi-permanent, strand-specific functionalization for extended monitoring. Both approaches generate uniform, mechanically robust coatings that maintain natural hair flexibility while preserving low impedance (~300–500 Ω at 1 kHz for bundles) and long-term stability. eHAIR operates not only as a passive conductor but also as an active organic electrochemical transistor (OECT). A device fabricated directly on conductive hair demonstrates volumetric ionic gating, peak transconductance up to 9 mS, and geometry-defined gain arising from intrinsic hair resistance, resulting in substrate-free common-source amplifiers. Improved signal quality compared to conventional Au/gel electrodes is confirmed in vivo in anesthetized rat EEG, with 3–5× higher spectral power in low-frequency bands and enhanced signal-to-noise ratios (28 dB vs. 16 dB) during baseline and epileptiform activity. Recordings are achieved without gels, or rigid hardware. Beyond transforming hair into an electrode, eHAIR redefines hair as an active electronic material, establishing a scalable, bio-integrated platform for neural monitoring and high-density electrophysiological recording.

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References

X. Strakosas et al., Metabolite-induced in vivo fabrication of substrate-free organic bioelectronics. Science 379, 795-802 (2023).

I. R. Minev et al., Electronic dura mater for long-term multimodal neural interfaces. Science

347, 159-163 (2015).

I. Uguz et al., Complementary integration of organic electrochemical transistors for front-end amplifier circuits of flexible neural implants. Science Advances 10, eadi9710 (2024).

Glass-like non-equilibrium dynamics in heavily doped polymer conductors

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Conducting polymers are mixed ionic–electronic conductors that are emerging candidates for neuromorphic computing, bioelectronics and thermoelectrics. However, fundamental aspects of their many-body correlated electron–ion transport physics remain poorly understood. Recently, we observed non-equilibrium transport signatures related to the interaction-driven formation of a frozen, soft Coulomb gap in the density of states, which opens up new opportunities for substantially enhancing the thermoelectric properties of conducting polymers.[1] Our preliminary work demonstrated that these non-equilibrium signatures are history-dependent and exhibit aging phenomena, indicating glass-like behaviour. However, a quantitative understanding of the most critical parameter, the relaxation time, is still lacking. In this study, we probe the time-dependent relaxation processes governing non-equilibrium charge transport in heavily doped polymers by systematically measuring relaxation time scales across a broad temperature range. We observe that the characteristic relaxation times increase with decreasing temperature following an Arrhenius-type trend, a hallmark of glass-like dynamics. These findings provide strong evidence for the existence of slow collective dynamics and emergent electronic glass states in heavily doped polymers. From the fundamental perspective, our work deepens the understanding of non-equilibrium phenomena in organic electronic materials and highlights doped polymers as a powerful model system for investigating glass-like physics. From the application perspective, our work offers insights into the design of high-performance devices that operate under non-equilibrium conditions.

Acknowledgements
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References
[1] DHL Tjhe#, X Ren#*, IE Jacobs#*, G D'Avino#*, H Sirringhaus#* et al., Nature Materials 23, 1712 (2024)

One-Pot Synthesis of Aqueous PEDOT-Based Conductive Inks via Sequential RAFT/Oxidative Polymerization.

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The rising demand for flexible and printable electronics has driven significant interest in π-conjugated polymers, in particular for poly(3,4-ethylenedioxythiophene) (PEDOT), which is traditionally stabilized by poly(styrenesulfonate) (PSS). For about ten years, our group has been investigating poly[4-styrenesulfonyl(trifluoromethylsulfonyl)imide] (PSTFSI) as a promising alternative polyelectrolyte, yielding PEDOT:PSTFSI dispersions with enhanced ionic conductivity, reduced acidity, and lower hygroscopicity.1-2 Although this polymer complex offers great potential in organic electronics, their synthesis still requires long reactions times (up to several days) and the use of toxic organic solvents with tedious intermediate purification steps, limiting their scalability and sustainability. Herein, we report an innovative aqueous one-pot synthesis of PEDOT:PSTFSI dispersion, by combining RAFT and oxidative polymerization in an aqueous one-pot process.3 This approach eliminates the need for harmful solvents and intermediate purifications, achieving full monomer conversion in less than 3 hours and excellent control over macromolecular structure of PSTFSI (30 to 300 kg mol-1 with Đ often below 1.1). Following the oxidative polymerization in a one-pot process, the resulting PEDOT:PSTFSI dispersions exhibit filamentous network morphologies, forming highly percolated conductive films upon printing, with charge conductivities up to 120 S cm-1. Not only this approach is faster and provides a precise control over macromolecular structure, but also aligns with six out of twelve principles of green chemistry : prevent waste, less hazardous synthesis, benign solvents, design for energy efficiency, use of renewable feedstocks and inherently benign chemistry for accident prevention. This scalable and sustainable route to obtain water-processable inks facilitates large-scale organic electronic processing, paving the way for the next generation of sustainable printed electronics.

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References

1. Hofmann, A. I. et al. Angew. Chem. Int. Ed., 54, 8506-8510 (2015).

2. Nugraha, I. M. et al. Adv. Science 11(46), 2409403 (2024).

3. Negny, F. et al. European Patent Application # EP25306689.8 (10 October 2025).

Selection rules and charge order pattern in BEDT-TTF κ-phase salts

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The salts of bis(ethylenedithio)-tetrathiafulvalene (BEDT-TTF) molecule and its variants play a central role among molecular quantum materials. The presence of itinerant electrons gives rise to a plethora of quantum phenomena, like superconductivity, charge fluctuations, charge-ordering, ferroelectricity, spin liquids state and so forth. Vibrational spectroscopy is an invaluable tool for the characterization of BEDT-TTF salts, due to the coupling to the electron system (e-mv coupling), that in dimerized salts, like those of the k-phase, give rise to strom IR bands, typically in the 1100-1300 cm -1 region. Some of these salts become superconductors, whereas some undergo a charge localization (charge order, CO), possibly ending in a ferroelectric state. The CO phase often occurs in the proximity of the superconducting phase, or may even coexist. Everyone so far has assumed that in k-phase the CO is within a dimer. However, intra-dimer CO implies loss of inversion center, so that infrared modes become Raman active and vice-versa. Therefore, if CO is intradimer, the strong IR e-mv induced bands should become Raman active, but none is found at the phase transition. I am proposing a change of paradigm: Different dimers bear a different average charge, the inversion center is maintained [1]. This is a rather indirect proof. Here I shall present additional evidences in support of my hypothesis.

References

[1] A. Girlando, Phys. Rev. B 110, 035101 (2024)

Thermal and Light-Induced Stability Study of a High-Efficiency Vacuum-Deposited Small-Molecule OPV Donor

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The long-term stability of organic photovoltaic (OPV) materials remains a major challenge, limiting device lifetime and reliability. Despite increasing interest in stability studies [1], systematic data under controlled stress conditions remain insufficient to fully understand the mechanism of how these materials respond to combined thermal and light exposure.

In this work, pure films of the efficient donor 2-((7-(5-(Di-p-tolylamino)thiophen-2-yl)benzo[c][1,2,5]thiadiazol-4-yl)methylene)malononitrile (DTDCTB) deposited by vacuum thermal evaporation were prepared and subjected to four controlled accelerated aging scenarios under encapsulated conditions: intense irradiation with LED light at room temperature, irradiation at elevated temperature, dark conditions at room temperature, and dark conditions at elevated temperature.

Preliminary UV–Vis results indicate that the material remains relatively stable under mild conditions, while changes in the absorption profile become more noticeable under thermal and illumination stress. FT-IR measurements suggest that these conditions may lead to variations in spectral features, pointing to possible structural or chemical modifications. Complementary characterization by NMR and fluorescence spectroscopy is being used to further probe these effects, providing insight into potential molecular-level degradation pathways and changes in emissive behavior.

As a next step, the material's stability will be evaluated directly in OPV devices by tracking the evolution of J–V characteristics under controlled stress conditions. These results are expected to contribute to a better understanding of degradation mechanisms and to guide strategies to improve device stability.

Acknowledgements
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References
N. Ahmad, J. Yuan and Y. Zou, Energy & Environmental Science 18, 5093-5158 (2025)

Thermally Activated Delayed Fluorescence Sensitized Blue Organic Light-Emitting Diodes

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Blue organic light-emitting diodes (OLEDs) remain a central challenge due to the trade-off between efficiency and operational stability. Thermally activated delayed fluorescence sensitized fluorescence (TSF) has emerged as a promising strategy to achieve near-unity exciton utilization while maintaining narrowband deep-blue emission. We investigate the thermodynamic and kinetic regulation of sensitized blue OLEDs to improve both efficiency and device lifetime. First, fully deuterated TADF sensitizers were developed to suppress high-frequency molecular vibrations, thereby reducing non-radiative decay and chemical bond dissociation. Devices incorporating deuterated emitters exhibited enhanced external quantum efficiency (EQE), prolonged operational lifetime, and improved color purity. Second, a delocalized electron distribution strategy was proposed to synergistically enhance thermodynamic robustness and excited-state kinetics. By increasing bond dissociation energy in the anionic state and accelerating reverse intersystem crossing (RISC), fragile bond cleavage and high-energy exciton annihilation were suppressed. The resulting TSF devices achieved record operational lifetimes among reported sky-blue and deep-blue systems. Finally, a phosphor-assisted TSF (pTSF) architecture was introduced to reduce efficiency roll-off and exciton annihilation. By modulating exciton dynamics through multi-sensitizer energy transfer, triplet exciton density was effectively lowered. The pTSF devices demonstrated a 1.6-fold improvement in operational lifetime and achieved state-of-the-art efficiency and critical current density for deep-blue OLEDs. These results establish a comprehensive framework for stabilizing blue TSF OLEDs through coordinated thermodynamic and kinetic control, providing practical guidelines for next-generation high-performance deep-blue devices.

References

T. Huang, et al. Enhancing the efficiency and stability of blue thermally activated delayed fluorescence emitters by perdeuteration. Nature Photonics, 2024, 18, 5, 516-523.

T. Huang, et al. Delocalizing electron distribution in thermally activated delayed fluorophors for high-efficiency and long-lifetime blue electroluminescence. Nature Materials, 23, 11, 1523-1530.

Atomic Layer Deposition of Ultrathin Topological Semimetals with Thickness-Dependent Resistivity

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As the device dimension continues being scaled down, conventional interconnect metals suffer from severe performance degradation at reduced thicknesses, motivating the search for alternative materials compatible with advanced integration schemes. Topological semimetals (TSMs) have recently emerged due to their unconventional transport behavior in the ultrathin regime. [1] For example, prior studies on NbP and TaP have shown that these Weyl semimetals exhibit robust metallic transport and suppressed resistance degradation. [2], [3] We recently published to Science, demonstrating that ultrathin non-crystalline NbP films exhibit unconventional resistivity scaling, reaching a room-temperature resistivity as low as 34 μΩ·cm at a thickness of 1.5 nm. [4] In this work, we demonstrate ultrathin TSM films deposited below 5 nm using atomic layer deposition (ALD) as a scalable and integration-friendly approach. Unlike standard ALD steps, we introduce an additional in-cycle chemical purge step to actively modulate the surface chemistry during film deposition, thereby establishing ALD process for ultrathin NbP. Compared to conventional metals, ultrathin TSM films exhibit favorable electrical transport characteristics with suppressed resistivity degradation upon thickness scaling. Resistivity values remain stable in the sub-5-nm regime, despite seedless deposition on 6-inch wafers at a low temperature of 170 °C. Post-deposition annealing further enhances structural ordering and improves electrical performance. Notably, these thickness-dependent transport characteristics persist even deposited on amorphous Si substrates, indicating the observed behavior is not reliant on the templates. These results highlight both the promise of ultrathin TSM films as a scalable interconnect material and the importance of interface engineering to fully realize its potential in nanoscale devices.

Acknowledgements
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References

I. K. Oh et al., IEEE International Interconnect Technology Conference (IITC), 1-3 (2025).

S.-Y. Xu et al., Science Advances 1, e1501092 (2023).

A. Bedoya-Pinto, ACS Nano 14, 4405-4413 (2020).

Effect of addition carbon nanotubes (MWCNTs) on the microstructure, mechanical properties and wetting of nanocomposites Sn-Bi/MWCNTs solder alloys

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Sn‒Bi solder alloys stand out as lead-free alternatives for low-temperature electronic applications; however, their use is still limited by the brittleness associated with Bi-rich phases and by challenges related to solderability. In this work, the influence of carbon nanotube (MWCNT) additions at different contents (0, 0.25, 0.50, and 1.00 wt%) on the microstructure, mechanical properties, and wetting behavior of Sn‒Bi alloys was systematically investigated. The samples were characterized by scanning electron microscopy coupled with energy-dispersive spectroscopy (SEM-EDS). Mechanical properties were evaluated by nanoindentation, while wetting behavior was analyzed by wetting force tests using a wetting balance. The results indicated that the unreinforced Sn‒Bi alloy exhibited a Vickers hardness of 26.3 HV and an elastic modulus of 30.8 GPa. The addition of MWCNTs promoted a progressive increase in these properties, reaching values of 28.1 HV and 34.3 GPa for the composition containing 1.00 wt% MWCNTs, accompanied by a reduction in plasticity from 93.37% to 88.12%. Microstructural analyses revealed modifications in the distribution of Bi-rich phases. Wetting tests indicated that the presence of MWCNTs influences the interfacial reactivity of the molten solder. The correlation between microstructure, mechanical properties, and wetting behavior allowed the identification of a MWCNT content range capable of balancing mechanical reinforcement and processability.

Acknowledgements
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References
B. Illés, O. Krammer, A. Géczy Introduction to surface-mount technology Reflow Soldering, Elsevier (2020), pp. 1-62, 10.1016/B978-0-12-818505-6.00001-7

A.H. Nobari, S. St-Laurent, Y. Thomas, A. Bouchemit, G. L'Esperance Performance of fine and ultra-fine lead-free powders for solder paste applications 2018 IEEE 68th Electronic Components and Technology Conference (ECTC), IEEE (2018), pp. 1942-1950, 10.1109/ECTC.2018.00291

T. Hu, Z. Li, G. Wu, S. Li, K. Ding, Y. Gao Effect of the solder powder size of Sn-Bi-Ag-In lead-free solder on the wettability and microstructure of Cu substrate Mater. Perform. Charact., 12 (2023), pp. 117-128, 10.1520/MPC20230003

Exciton Dynamics Modulation in Conjugated Terpolymers: The Role of Fluorescent Pendant Groups

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This work investigates the incorporation of fluorescein octyl ester (FOE) as a fluorescent side group in benzodithiophene-based donor–acceptor terpolymers as a strategy to regulate exciton dynamics without substantially perturbing frontier orbital energies. Three FOE-containing terpolymers (P2-iIa-c) were systematically compared with a non-functionalized analogue (P1-iI). FOE incorporation increased glass transition temperatures, indicating restricted segmental mobility and greater conformational constraints within the conjugated backbone. Optical characterization revealed distinct absorption evolution, shortened fluorescence lifetimes, and spectral overlap consistent with intramolecular energy-transfer processes (FRET-like) from FOE units to lower-energy backbone segments, with estimated transfer efficiencies of 60–65%. Cyclic voltammetry showed only minor HOMO variations while preserving LUMO energies, confirming that side-chain functionalization primarily modulates photophysical behavior rather than significantly altering electronic structure. Under bilayer photovoltaic conditions, FOE-containing terpolymers exhibited systematically enhanced photocurrent generation relative to P1-iI, attributed to improved exciton generation, migration, and redistribution processes. Additionally, FOE incorporation influenced polymerization behavior by limiting chain growth and modifying segmental composition, progressively enriching BDT-BTzFOE segments. Overall, these findings demonstrate that fluorescent side-chain engineering provides an effective strategy for simultaneously tuning backbone rigidity, segmental distribution, and excitonic processes in conjugated polymers while preserving their intrinsic electronic structure, offering new opportunities for the rational design of advanced photovoltaic materials.

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References
I.A. Jessop, J. Cutipa, Y. Perez, C. Saldias, D. Fuentealba, A. Tundidor-Camba, C.A. Terraza, M.B. Camarada, F.A. Angel, New Benzotriazole and Benzodithiophene-Based Conjugated Terpolymer Bearing a Fluorescein Derivative as Side-Group: In-Ternal Forster Resonance Energy Transfer to Improve Organic Solar Cells, Int J Mol Sci 23(21) (2022)

Sensitive Piezoelectric Layer with Additives and Electrospun PVDF Nanofibers

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The beta phase of Poly(vinylidene fluoride) (PVDF) is widely recognized for its highly ordered and stable crystalline structure. In this phase, PVDF molecules arrange themselves regularly, forming a compact and uniform matrix that imparts significant piezoelectric properties, thermal stability, and superior mechanical strength. PVDF nanofibers produced via the electrospinning technique exhibit a well-defined crystalline structure, predominantly in the beta phase, making them highly suitable for advanced applications in nanotechnology, electronics, and biomedicine. Electrospinning allows for precise control over the morphology and orientation of the fibers, adjusting their characteristics to meet the specific needs of diverse applications, such as pressure sensors, energy harvesters, and specialized biomedical devices. This study aims to enhance the effectiveness of electrical current storage and generation, as well as improve the sensitivity of pressure sensors. During the experimental procedure, the solution was inserted into a 3.0 mL syringe within an infusion pump, with the flow rate set to 0.5 mL/h and the needle positioned at a distance of 15 cm from the collector. The solution was injected into a rotating collector at 300 rpm, maintaining the relative humidity at a constant 70%. The total concentration of PVDF and solvents was 15% (w/w). The results were thoroughly analyzed by SEM microscopy to observe the linearity, continuity, and thickness of the fibers. Using FTIR spectra, it was possible to calculate the relative percentage of the most predominant crystalline phase, comparing the proportion between the phases of PVDF in the electrospun nanofibers. XRD/XRF indicated the specific crystalline phases identified, along with their chemical elements. Finally, the results of DC electrical conductivity tests will be used to demonstrate the piezoelectricity of the developed material.

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References

MENG, F. et al. Applied Surface Science, v. 619, p. 156782, 2023.

ZHANG, H. et al. Journal of Materials Science & Technology, v. 184, p. 112-125, 2025.

SANTOS, R. L. et al. Nano Energy, v. 131, 110542, 2025.

Study of optical and structural properties of columnar liquid crystal films produced by drop-casting, spin-coating and blade-coating

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Liquid crystals (LC) are materials that exhibit intermediate phases between crystalline solids and isotropic liquids and are promising organic semiconductors due to their self-organization and the possibility of molecular alignment on electrodes, enhancing charge carrier mobility [1-3]. Within this framework, this work investigates how different deposition methods (spin coating, blade coating, and drop casting) affect the optical, structural, and morphological properties of NiPc (nickel phthalocyanine) and D2 (perylenetetracarboxylic diimide) films, both columnar liquid crystals at room temperature. For preparation, NiPc was dissolved in THF (tetrahydrofuran) and D2 in chloroform, ensuring suitable solutions for deposition. Techniques such as polarized optical microscopy, X-ray diffraction, UV-vis spectroscopy, and photoluminescence were employed to investigate the morphological, structural, and optical properties of the films. Preliminary results show that NiPc films do not exhibit significant changes depending on the deposition method, while D2 films demonstrate photoluminescent response strongly dependent on the deposition method, with higher quantum yield in drop casted and lower in blade coated films. Next steps include increasing the concentration of the solution to produce thicker films and applying atomic force microscopy (AFM) to correlate morphology with the deposition methods.

References

Gupta, R. K., Manjuladevi, V., Karthik, C. Choudhary, K. Thin films of discotic liquid crystals and their applications. Liq. Cryst. 43, 2079–2091 (2016).

C. Ruiz, E.M. García-Frutos, G. Hennrich, B. Gómez-Lor, J. Phys. Chem. Lett. 3, 1428–1436 (2012)

J. Eccher, W. Zajaczkowski, G.C. Faria, H. Bock, H. von Seggern, W. Pisula, I.H. Bechtold, ACS Appl. Mater. Interfaces 7, 16374–16381 (2015)

Theory for synthetic electronic materials: from transport and thermoelectric conversion to light-emitting

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Synthetic electronic materials are distinctly different from conventional inorganic semiconductors or metals due to the structural flexibility and intrinsic impurity/disorder. The carrier transport behaviors cover from hopping, phonon-assisted current, transient localization and bandlike [1]. Under doping, there appear polaron/bipolaron stucture, which can lead to "abnormal Seebeck effect", namely, upon increasing temperature, the Seebeck coefficient (transport entropy) could even decrease [2] and even sign change, namely, heavily p-doped polymer could present negative Seebeck coefficient due to the strong electron correlation effect. We also demponstrate there can appear Seebeck coefficient anisotropy which has been observed in experiments but never been understood before. We further present our rate theory for OLEDs [3] and machine learning strategy to design light emitting molecules with inverted singlet-triplet excited state structure [4] and high g-value circular polarized luminescent (CPL) molecules and aggregate [5]. We finally investigate the synthesizability for ML.

References

[1] Z. Shuai, Nature Mater. 2023, 22, 1277

[2] Y. F. Ge, Appl Phys Lett 2021, 118, 123301

[3] Z. Shuai and Q. Peng, Phys Reports 2014, 537, 123

[4] R. Mahaan and Z Shuai, J Phys Chem Lett 2026, 17, 6233

[5] R. Mahaan, W T Li, Z. Shuai, J Phys Chem C 2026, 130, 7812

Adaptive Aromaticity and Its Application to Singlet Fission

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Keywords: Aromaticity, Singlet Fission, DFT calculations, Excited State

Adaptive aromaticity has attracted substantial attention due to its unconventional two-state aromaticity in both the lowest singlet state (S_0) and the lowest triplet state (T_1) and its application to singlet fission.[1-2] This concept denotes two-state aromaticity and thus stands in marked contrast to the traditional one-state aromaticity governed by the Hückel and Baird rules. Here, we carry out a comprehensive investigation on a series of pyrrole derivatives by density functional theory (DFT) calculations and machine learning (**Scheme 1**).[3] Various aromaticity indices including HOMA, NICS, EDDB, and MCI suggest that the pyrrole rings in these derivatives show adaptive aromaticity when the other ring of bicyclic systems has weaker (or comparable) aromaticity than the pyrrole ring among these pyrrole derivatives, which could be considered as a sacrificial reagent strategy to achieve adaptive aromaticity of these pyrrole rings. In contrast, when the other ring such as the phenyl ring has stronger aromaticity than the pyrrole ring, it cannot be sacrificed to achieve adaptive aromaticity of the pyrrole rings. More interestingly, a singlet fission chromophore is predicted when the other ring is an antiaromatic borole among these pyrrole derivatives. Additionally, principal component analysis (PCA, one of the most commonly used unsupervised machine learning algorithms) suggests that $\Delta NICS(1)_{zz}$ ($NICS(1)_{zz}(S_0) - NICS(1)_{zz}(T_1)$) of the other ring in these pyrrole derivatives can be an important factor in predicting $E(T_1)$ values, which is also supported by a strong correlation ($R^2 = 0.98$) between $\Delta NICS(1)_{zz}$ and $E(T_1)$. All these findings provide an alternative idea for the design of singlet fission chromophores.

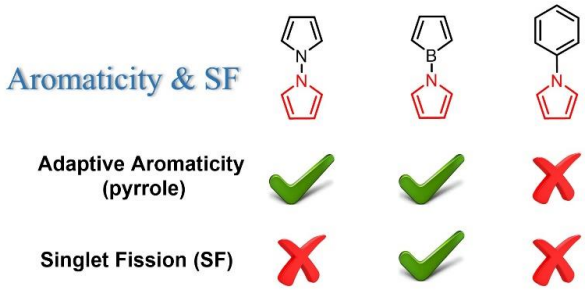


Figure 1: The proposed sacrificial reagent strategy to achieve adaptive aromaticity in the pyrrole rings

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References:

[1] T. Shen, et al., *J. Am. Chem. Soc.*, **141**, 5720 (2019).
[2] L. Wang, et al., *J. Am. Chem. Soc.*, **142**, 10235 (2020).
[3] Q. Deng, et al., *Org. Chem. Front.*, **13**, 484 (2026).

Controlling spin by materials design in light-emitting applications: A computational perspective

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Keywords: Light-emitting materials, Thermally Activated Delayed Fluorescence, Radicals, Inverted Singlet-Triplet gap materials, Multi-Resonant

OLEDs efficiencies are tightly bound with the spin statistics of charge recombination which for conventional fluorescent materials results in a balance of one emissive singlet to three lost to heat triplets. Therefore, the internal quantum efficiency (IQE) is limited to 25 percents in this class of materials. Over the last years, different strategies to design fully organic light-emitting materials including thermally activated delayed fluorescence (TADF), inverted singlet-triplet gap materials (INVEST) as well as doublet radical emitters have been proposed allowing in theory to reach 100% IQE. In this communication, we will discuss the optoelectronic properties of these different classes of materials based on computational considerations. Especially:

- We will discuss how doped triangle-shaped molecules can lead to (i) concomitant narrow emission, high quantum yield of emission and small singlet-triplet gap ΔE_{ST} resulting in a whole new generation of TADF emitters, the multi-resonant TADF emitters[1] and to (ii) inverted ΔE_{ST} (INVEST) materials leading potentially to a downwards energy RISC.[2,3,4]
- We will show how the optoelectronic properties of organic radical materials can be tuned and lead to either red emitters for OLEDs with IQE up to 100 percents or materials with optically accessible high spin state for quantum information applications [5]

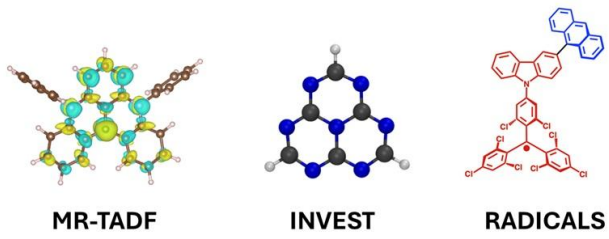


Figure 1: OLEDs materials

References:
[1] A. Pershin et *al.* Nat. Commun. **10**, 597 (2019).
[2] G. Ricci et *al. ChemPhysChem* **22**, 553 (2021).
[3] J. Sanz-Rodrigo et *al. J. Phys. Chem. A* **125**, 513 (2021).
[4] G. Ricci, J. C. Sancho-García, Y. Olivier, *J. Mater. Chem. C* **10**, 12680 (2022).
[5] S. Gorgon et al., Nature **620**, 538 (2023).

Defects and Degradation in Organic Semiconductors – New Methods of Detection to Variables Influencing Degradation

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Keywords: Photoelectron spectroscopy, stability, trap states, doping, optical properties

Organic semiconductors (OSCs) are attractive for myriad applications, from biosensors and neuromorphic computing to electrochromic devices and light emitting diodes. While molecular OSCs have achieved major commercial success in organic light emitting diodes, this level of commercialization has not yet reached other device types or polymeric OSCs. For conjugated polymers (CPs), the lack of widespread commercialization can largely be attributed to two interrelated factors: purity and stability. Without consistent high purity, reproducibility is difficult to obtain, and without high stability, commercialization options are extremely limited. Furthermore, purity and stability go hand in hand, with low purity materials leading to rapid material and device degradation. Despite the importance of material purity and reducing degradation, research in these areas is limited.

To understand and probe material purity and degradation, we need robust methods for detecting intra-gap defect states (DS). These DS are harmful impurities (from chemical defects in the OSC to residual catalyst) that can act as charge traps to limit transport, hurt reproducibility, and catalyze degradation processes. Degradation processes can also result in formation of DS that can cause drastic decreases in device performance. To detect DS in organic semiconductors, we have developed a variable energy ultraviolet photoemission spectroscopy (VE-UPS) instrument, which can probe defect states that are present in parts per million concentrations relative to the HOMO or LUMO states. I will discuss the basics of VE-UPS and its application to understanding defects and degradation in molecular OSC and CPs. For example, we have applied VE-UPS to probe defect states that arise during degradation upon exposure to different stressors. Additionally, we have applied VE-UPS to doped organic OSCs to determine how doping impacts the density of occupied DS.

Degradation of molecular OSCs and CPs will be dependent on numerous variables, from environmental stressors to the structure and morphology of the CP. With the increasing interest in doped CPs for their application to thermoelectrics, organic electrochemical transistors, electrochromic devices, and injection layers in light emitting diodes and solar cells, it is important to understand the variables influencing stability of doped CPs. In this work, we investigated the stability of a series of electrochemically doped CPs at two different doping levels with counterions of varying size under exposure to different stressors. From this set of experiments, we show that larger counterions lead to improved stability, stability in the doped state increases as the ionization energy of the CP decreases, and humidity has a large impact on degradation rates.

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From Spherical to Flattened Linear Structure: Exploring Minimal Units of Electron-Accepting Conjugated Hydrocarbons

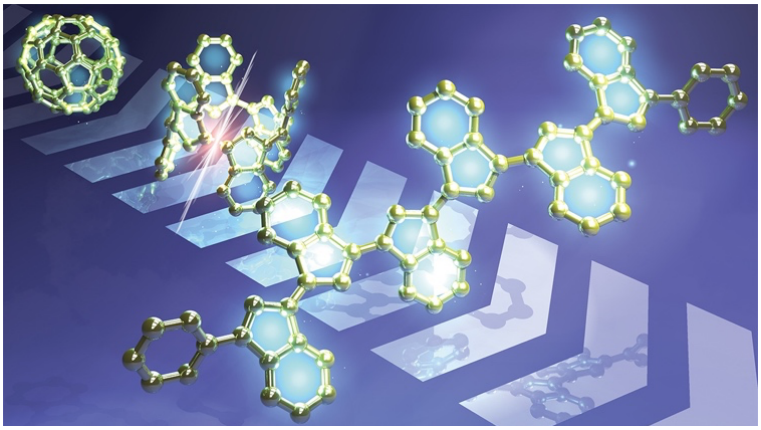
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Keywords: electron acceptor, conjugated hydrocarbon, fullerene, conjugated polymer

Fullerenes have long attracted attention as architecturally unique and electronically intriguing molecular systems. Among their diverse characteristics, their outstanding electron-accepting properties, including low-lying LUMO levels and exceptional stability toward multi-electron reduction, are particularly notable. Understanding the minimal structural units responsible for these properties could offer key insights into the origin of their electron affinity and inform new design principles for organic electron acceptors. In this context, we have focused on the use of pentafulvalene as a central building block. Pentafulvalene consists of two cyclopentadiene rings cross-conjugated via an exocyclic double bond, a subunit found in fullerenes. Building on this concept, we have recently developed linear π-conjugated oligomers incorporating dibenzopentafulvalene as repeating units.[1] These oligomers, featuring pentagonal connectivity analogous to that of C_{60} but without the curvature or rigidity, exhibit notable stability toward multi-electron reduction and relatively high electron affinity. In this presentation, I will present an overview of this design strategy and highlight recent developments in the synthesis and characterization of these oligomers and relevant molecular systems.[1–4]



References:
[1] A. Fukazawa et al., *Nat. Commun*, **14**, 2741 (2023).
[2] A. Fukazawa et al., *Chem. Eur. J.*, **29**, e202300181 (2023).
[3] A. Fukazawa et al., *manuscript in preparation*.
[4] A. Fukazawa et al., *Chem. Sci.*, **17**, 3005 (2026).

Impurities in Arylboronic Esters Induce Persistent Afterglow

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Abstract

Several recent reports suggest that arylboronic esters can exhibit room temperature phosphorescence (RTP), an optical property that is desirable for applications in security printing, oxygen sensing, and bioimaging. These findings challenged the fundamental notion that heavy elements or changes in orbital symmetry were required for intersystem crossing to occur in organic compounds. As we had not observed long afterglow in the many arylboronic esters we had synthesized over many years, we suspected that the RTP observed in these systems had a simpler explanation: the materials reported were impure. Herein, we synthesized numerous arylboronic esters that were previously reported to show RTP, and carefully purified them by column chromatography, recrystallization, and sublimation. We re-examined their photophysical properties alongside single-crystal X-ray diffraction analysis and detailed theoretical studies. While several of these compounds showed long afterglows as crude products, none of them showed persistent RTP after careful purification. We also successfully isolated the impurity 4-amino-3,5-bis(pinacolatoboryl)benzonitrile (2), identifying it as the impurity responsible for inducing delayed fluorescence in 3,5-bis(pinacolatoboryl)benzonitrile (1). Doping 1 with 1.0 mol % 2 led to a persistent afterglow with a lifetime of 67 ms, which is mediated by a dimer charge transfer state. Our findings call for a re-examination of previous studies reporting RTP from arylboronic esters, highlight the importance of careful purification in photophysical research, and provide a practical strategy for designing organic materials with a long afterglow.

Innovation in Molecular & Thin Film Engineering for Stretchable & Functional Electronics

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Skin-like soft electronic devices and stretchable conducting films are a prime necessity for future stretchable and wearable electronics. We deposited highly conducting poly(3,4 ethylenedioxythiophene):Tosylate (PEDOT:Tos) films on extremely stretchable styrene-ethylene-butylene-styrene (SEBS) as well as biocompatible seafood waste derived Chitosan substrates via vapor phase polymerisation (VPP) for charge transport study including their use in organic electrochemical transistor (OECT) devices. [1,2] Such devices hold great potential for highly sensitive wearable biosensors & medical device technology. Our newly developed pyridine flanked diketopyrrolopyrrole (DPPPy) end capped with thienyl naphthalimide n-type small molecule DPPPy-C-Si-TN together with SEBS blend show a high electron mobility of 0.322 $cm^2 V^{-1} s^{-1}$. [3] We also synthesized a series of high mobility inherently stretchable polymers based on furan/thiophene/selenophene/pyridine flanked diketopyrrolopyrrole (DPP), comprising, without, with a non-conjugated spacer in their backbone and cyano substituted thienyl-vinylene-thienyl polymers for high performance stretchable OFETs (with highest hole mobility of 1.8 cm2/Vs and electron mobility 2.0 cm2/Vs) and these devices were further demonstrated for advanced stretchable logic circuits, photodetectors & artificial neuromorphic visualizer e-Skin applications.[3, 4, 5.] Some of the recent work on the novel conjugated polymers with radicals for the thermoelectric and other functional devices will be presented. [6, 7]

References:

1. V. Sethumadhavan, E. Switalska, M. Shahbazi, Y. Li, K. Zuber, T. Wang, J. Alarco, D. R. Evans, P. Sonar. **Adv. Electron. Mater**., 2024, 2300602.
2. C. Khamhanglit, T. Li, V. S. Sethu Madhavan, J. McDonald, E. Switalska, A. Sun, I. Prasadam, Y. T. Gu, D. R. Evans, W. L. Leong, P. Sonar, **Small Structures**, 2400642.
3. K. Kranthiraja, V. Sethumadhavan, S. Kumagai, Y. Xu, A. Erhardt, C. R. McNeill, S. Manzhos, J. Takeya, and P. Sonar, **Adv. Electron. Mater.** 2024, 2400614.
4. R. Kothandaraman, W. He, K. Kranthiraja, S. Manzhos, C. R. McNeill, Y. Li, K. Fairfull-Smith, T. Michinobu, P. Sonar "**Adv. Mater. Techn,** 2401518.
5. Manuscript submitted to **Communication Materials** and **Nature Electronics**
6. Manuscript submitted to **Nature Communication**
7. Manuscript under preparation

Organic Bulk Heterojunction Semiconductors for Photocatalysis and Solar Fuels

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DNŜŜY KèŘN2ƎŜyΣ LJN2ŘdzÕŜŘ ŦN2Y ǿI·ŭŜN dzăλyƎ NŜyŜǿI·ōfŜ ŜyŜNƎèΣ λă ŜÈLJŜŎŭŜŘ ŭ2 ōŜŎ2Y'Ŝ I· LJN2Y'λySyŭ ŦdzŭdzNŪŜ ŦdzŜfΣ LJN2ØλŘλyƎ ŎfŜI·yΣ ŎI·N¤ō2Y' ŦNŪŜŜ ŜyŜNƎè Ŧ2N I· ǿλŘŜ NI·yƎŜ 2Ŧ λyŘdzăŭNλI·f I·LJLJfλÕI·ŭλ2yãΦ Lŭ ÔI·Y' I·fă2 LJN2ØλŘŜ Õ2Y'LJfŜY'Ŝyŭ I·N¤è ŜyŜNƎè ăŭ2NI·ƎŜ λY' Õ2Y'ōλyl·ŭλ2Y' ǿλŭK λyŭŜNY'λŭŭŜyŭ ă2fI·N ŜyŜNƎèΦ I2ǿŜØŜNΣ Õ2Y'LJŜŭλŭλØŜ ŜÕ2y2Y'λÕ ă2fI·N ƎŜyŜNI·ûŜŘ KèŘN2ƎŜY' LJN2ŘdzÕŭλ2Y' 2Y' I· fI·NƎŜ ăÕI·fŜ NŜY'I·λyã ÕKI·ffŜyƎλyƎΦ hyŜ LJN2Y'λăλyƎ I·LJLJN2I·ÔK λă LJK2ŭ2ÕKŜY'λÕI·f ǿI·ŭŜN ăLJfλŭŭλyƎΣ dzăλyƎ fλƎKŭ I·ōă2NōλyƎ yl·y2LJI·NŭλÕfŜ ăŜY'λÕ2yŘdzÕŭ2Nă ŭKI·ŭ ÕI·Y' ŘNλØŜ NŜŘ2È NŜI·Õŭλ2yã 2Y' ŭKŜλN ădzNŦI·ÕŜΦ ¢NI·Řλŭλ2yl·ffèΣ ǿλŘŜ ōI·yŘƎI·LJ λy2N¤I·yλÕ ăŜY'λÕ2yŘdzÕŭ2Nă KI·ØŜ ōŜŜY' dzăŜŘ Ŧ2N LJK2ŭ2ÕI·ŭI·fèŭλÕ I·LJLJfλÕI·ŭλ2yãΦ I2ǿŜØŜNΣ ŭKŜăŜ Y'I·ŭŜNλI·fă I·fY'2ăŭ ŜÈÕfdzăλØŜfè I·ōă2NōÇ ±fλƎKŭ ǿKλÕK 2yfè ÕI·NNλŜă I· ăY'I·ff ŦNI·Ôŭλ2Y' ó₣ƥ̂ú 2Ŧ ă2fI·N ŜyŜNƎèΣ fλY'λŭλyƎ ŭKŜNN ŜŦŦλÕλŜyÕè¢ Ly' ŭKλă LJNŜăŜyŭI·ŭλ2yΣ ŭKŜ ŘŜØŜf2LJY'Ŝyŭ 2Ŧ LJK2ŭ2πÕI·ŭI·fèăŭă ŦI·ōNλÕI·ŭŜŘ ŦN2Y' 2NƎI·yλÕ ăŜY'λÕ2yŘdzÕŭ2NăΣ ÕKŜY'λÕI·ffè ŭdzyŜŘ ú2 I·ōă2Nō ăŭN2yƎfè ŭKN2dzƎK2dzŭ ŭKŜ ¦±πØλăλōfŜ ăLJŜÕŭNdzY' ǿλff ōŜ ŘλăÕdzăăŜŘ ² Ŝ ŘŜY'2yãŭNI·ŭŜ I· fI·NƎŜN ă2fI·N ŭ2 KèŘN2ƎŜy' ŜŦŦλÕλŜyÕè ŭKI·y' ŭNI·Řλŭλ2yl·f λy2NƎI·yλÕ LJK2ŭ2ÕI·ŭI·fèăŭăΣ I·ÕKλŜØŜŘ ǿλŭK 2N¤I·yλÕ ăŜY'λÕ2yŘdzÕŭ2N yl·y2LJI·NŭλÕfŜă ŭKI·ŭ Õ2yŭI·λy' I·y' λyŭŜNyl·f Ř2y2NNkI·ÕÕŜLJŭ2N KŜŭŜN2ƨdzyÕŭλ2y' ōŜŭǿŜŜy' ŭǿ2 2N¤I·yλÕ ăŜY'λÕ2yŘdzÕŭ2Nă ǿλŭK I· ûèLJŜ LL ŜyŜNƎè fŜØŜf 2ŦŦăŜŭ¢KŜ Ř2y2NkI·ÕÕŜLJŭ2N KŜŭŜN2ƨdzyÕŭλ2y' ƎN¤Ŝl·ûfè λY'LJN2ØŜă ÕKI·NƎŜ ƎŜyŜNI·ûλ2y' ǿλŭKλy' ŭKŜ yl·y2LJI·NŭλÕfŜăΣ ǿKλÕK λy' ŭdzNy' ƎN¤Ŝl·ûfè λY'LJN2ØŜă ŭKŜN KèŘN2ƎŜy' LJN2ŘdzÕŭλ2y' ŜŦŦλÕλŜyÕè² Ŝ ŘŜY'2yãŭNI·ŭŜ I· ădzōăŭl·yŭλI·f λyÕNŜI·ăŜ λy' ŭKŜ KèŘN2ƎŜy' LJN2ŘdzÕŭλ2y' ŜŦŦλÕλŜyÕè ōè ŭdzyλyƎ ŭKŜ yl·y2LJI·NŭλÕfŜ Õ2Y'LJ2ăλŭλ2y¢ ² Ŝ I·fă2 2ōăŜN¤ØŜ ŭKI·ŭ ŭKŜ KλƎK ŜŦŦλÕλŜyÕè 2Ŧ ŭKŜăŜ y1·y2LJI·NŭλÕfŜă 2NλƎλyl·ŭŜă FN2Y ŭKŜλN I·ōλfλûè ú2 ƎŜyŜNI·ûŜ ŜÈÕŜLJŭλ2yl·ffè f2yƎπfλØŜŘ NŜI·ŎŭλØŜ ÕKI·NƎŜă dzLJ2y' λffdzY'λyl·ûλ2yΣ λyÕN¤Ŝl·ăλyƎ ŭKŜλN fλ]ŜfλK22Ř ŭ2 LJI·NŭλÕλLJI·ŭŜ λy' I· LJK2ŭ2ÕI·ŭI·fèŭλÕ NŜI·ŎŭλØŜ Ly' I·ŘŘλŭλ2yΣ ǿŜ ǿλff ŘλăÕdzăă ă2fdzŭλ2yπ LJN2ÕŜăăI·ōfŜΣ fλyŜI·N Õ2y¢dzƎI·ûŜŘ LJ2fèY'ŜNă 2Ŧ λyŭNλyãλÕ LJ2N2ăλûè Ŧ2N ƎI·ă LJKI·ăŜ ÕI·N¤ō2y' ŘλƎÈλŘŜ LJK2ŭ2NŜŘdzÕŭλ2yΦ I λƎKfλƎKŭλyƎ ŭKŜ LJ2ûŜyŭλI·f 2Ŧ LJN2ÕŜăăI·ōfŜ LJ2fèY'ŜNă 2Ŧ λyŭNλyãλÕ LJ2N2ăλûè Ŧ2N dzăŜ λy'ŭKŜ ƎI·ă LJKI·ăŜ LJK2ŭ2NŜŘdzÕŭλ2y'2Ŧ ÕI·N¤ō2y'ŘλƎÈλŘŜ ŭ2ǿI·NŘă ă2fI·N ŦdzŜfă¢

Spectroscopic proof of inversion of the lowest singlet and triplet energy states in the heptazine $HzTFEX_2$.

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Keywords: Singlet triplet state inversion

We will present evidence that $HzTFEX_2$ [1] has a long lived phosphorescence emission from the T_1 state, with a 0-0 peak at 425 nm and band shape nearly identical to monomer fluorescence, giving an inverted singlet triplet gap of 110±20 meV in frozen toluene at 2μM. Importantly we give a full set of measurements that support the possibility that phosphorescence from an inverted triplet state can be observed. Relatively strong anti-Kasha S_2 emission indicating slow internal conversion from S_2 to S_1. The S_2 S_1 energy gap is large, 0.85 eV, and as the $HzTFEX_2$ is rigid, there is not crossing of the S_2 and S_1 energy surfaces and vibronic coupling is weak. Single crystals measurements indicate S_2 and S_1 orbitals are orthogonal. Phosphorescence is only observed when we excite into the S_2 state, and thus propose that ISC/rISC predominantly occurs in the S_2 state. Exciting into S_1 yields no measurable phosphorescence so endothermic $S_1 \rightarrow T_1$ rISC is suppressed because of very weak vibronic coupling at low temperatures.

Excimers and dimers dominate most the observed photophysics. In dilute frozen 2-MeTHF solution, having a very low excimer content, we estimate that the PLQY reaches near unity because excimer formation is supressed. This points to negligible excited state loss by internal conversion and non-radiative decay through vibrational channels, supporting the notion that vibronic coupling in $HzTFEX_2$ is highly ineffective, especially in the S_1 and T_1 manifolds.

We observe hipsochromic solvatochromic effects in $HzTFEX_2$, even though the S_1 state is of ππ* character. We resolve this through comparison to previous work on molecules containing sp^2 hybridised nitrogen atoms within a conjugated structure, where the ground state is strongly localised due to the participation of the localised nitrogen lone pair electrons in the π orbitals, but the excited state is a delocalised π* state. In this situation the transition energy is sensitive to solvent polarizability. In this picture the excited delocalised electron is highly decoupled from its localised hole leading to very weak electron hole interactions, i.e. small or negative electron exchange energies.

References

[1] N. Aizawa et al., Nature **609**, 502, 2022

Squaraine dyes: from chiral aggregates to single-component photodetectors

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Squaraine dyes are a promising family of organic dyes for functional applications. Circular dichroism spectra of aggregates of squaraine dyes decorated with chiral groups, [1] supported by 2D-vis spectra of relevant films are analysed in terms of an essential state model, accounting for both intermolecular electrostatic interactions and intermolecular charge-transfer interactions, solving a controversy in the literature. The same model is applied to rationalize the intriguing observation of photocurrent generation in single component films of a NIR squaraine dye, recently exploited to build an efficient single-component active material photodetector. [2] The comparison of the behavior of pristine and annealed films, showing different amounts of crystalline and amorphous phases, is particularly informative, bringing us to the conclusion that field-assisted photoinduced generation of charges mainly occurs in the amorphous phase. The proposed analysis offers a sound interpretative framework for the puzzling and technologically relevant phenomenon of photoinduced charge separation in single-component molecular thin films. Specifically, we identified the high degree of electrostatic disorder characteristic of the amorphous phase of squaraine dyes as the driving force of the process. [3]

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References

Giavazzi, D.; Schumacher, M. F.; Grisanti, L.; Anzola, M.; Di Maiolo, F.; Zablocki, J.; Lützen, A.; Schiek, M.; Painelli, A. A Marvel of Chiral Squaraine Aggregates: Chiroptical Spectra beyond the Exciton Model. J. Mater. Chem. C 2023, 11 (24), 8307–8321.

Hu, W.-H.; Nüesch, F.; Giavazzi, D.; Jafarpour, M.; Hany, R.; Bauer, M. Squaraine Dyes for Single-Component Shortwave Infrared-Sensitive Photodiodes and Upconversion Photodetectors. Adv. Opt. Mater. 2024, 12 (10), 2302105. https://doi.org/10.1002/adom.202302105.

D. Giavazzi, M. Bauer, M. Diethelm, J.P. Ferreira Assunção, R. Hany, W-H Hu, M. Jafarpour, A. Neels, F. Nüesch, D. Sapalidis, B.F.B. Silva, A. Painelli, Photoinduced charge separation in single-component squaraine films: the key role of electrostatic disorder, submitted.

The influence of non-covalent contacts on stability in boron-containing donor-acceptor compounds designed to feature TADF

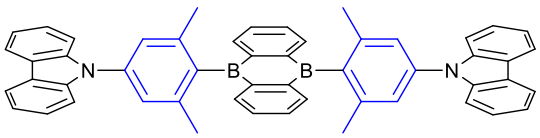
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Keywords: synthetic materials chemistry, molecular structure, donor-acceptor molecules, TADF

Non-covalent interactions are highly important and often overlooked phenomena in materials chemistry. Hydrogen bonding, π-π associations and heteroatom interactions represent some of the modes that provide molecular orbital overlap within and between molecules, resulting in observed short contacts between molecular units. These non-covalent interactions can dictate molecular conformation [1], and/or establish long-range order and connectivity to promote bulk properties, such as conductivity, in molecular materials [2]. Molecular conformation is a highly important factor in the design of donor-acceptor materials for thermally activated delayed fluorescence (TADF). Manipulation of ground and excited state structures allows one to vary the energy of the charge-transfer (CT) states to aid in efficient reverse intersystem crossing (rISC), by establishing a very low energy barrier between singlet and triplet states. Molecular conformation is therefore key in providing optimal CT geometries. As an example, weakening the π-conjugated link between donor and acceptor units can be achieved through a twisted geometry that disrupts p-orbital alignment within the conjugated bridge and keeps donor and acceptor units separated. The compound **CzDBA**, shown below, uses steric properties to accomplish this, and the material gives outstanding performance as a TADF emitter in OLED devices (37.8% EQE with an efficiency roll-off of 0.3% at 1,000 cd m^{-2}) [3]. In our work, we have taken analogous compounds with heteroatoms replacing the methyl groups in the π-bridge (shaded blue below), to see if X···B interactions (where X is a heteroatom), have any effect on the photophysical properties of these donor-acceptor molecules. We report here the synthesis, physical and photophysical properties, and conformational analysis of analogues of **CzDBA**.



CzDBA

References

[1] G. Conboy, H. J. Spencer, E. Angioni, A. L. Kanibolotsky, N. J. Findlay, S. J. Coles, C. Wilson, M. B. Pitak, C. Risko, V. Coropceanu, J.-L. Brédas and P. J. Skabara, *Mater. Horiz.*, 2016, **3**, 333-339.

[2] J. Cameron, A. L. Kanibolotsky and P. J. Skabara. *Adv. Mater.*, 2024, **36**, 2302259.

[3] T. L. Wu, M. J. Huang, C.C. Lin, P. Y. Huang, T. Y. Chou, R. W. Chen-Cheng, H. W. Lin, R. S. Liu and C. H. Cheng, *Nat. Photonics* 2018, **12**, 235–240.

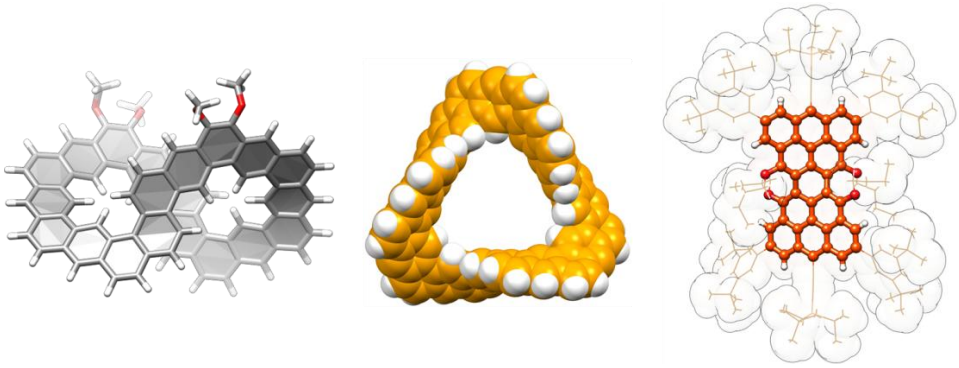
Topological Molecular Carbons

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I will present our latest research works on graphene-based molecules[1] and topological molecular carbons,[2] focusing on their synthetic chemistry, edge-dependent electronic properties, aromaticity, open-shell character, chirality, π-magnetism, and potential quantum properties. I will also address the perspectives and challenges in this field.



References:

[1] (a) T. Jiao et al., *Nat. Synth*. **2023**, *2*, 1104–1115; (b) Y. Zou et al., *Angew. Chem. Int. Ed.* **2023**, e202301041; (c) T. Shen et al., *Angew. Chem. Int. Ed.* **2023**, e202304197; (d) T. Shen et al., *Angew. Chem. Int. Ed.* **2023**, e202311928; (e) Y. Zou et al., *J. Am. Chem. Soc.* **2024**, *146*, 27293–27298; (f) S. Song et al., *Nat. Chem.* **2024**, *16*, 938–944; (g) T. Shen et al., *Angew. Chem. Int. Ed.* **2024**, e202410828; (h) T. Jiao et al., *Nat. Chem.* **2025**, *17*, 924–932; (j) L. Jiao et al., *J. Am. Chem. Soc.* **2025**, *147*, 9415–9423; (k) Z. Sun et al., *Angew. Chem. Int. Ed.* **2026**, DOI: 10.1002/anie4322934.

[2] (a) W. Fan et al., *J. Am. Chem. Soc.* **2021**, *143*, 13908; (b) W. Fan et al., *J. Am. Chem. Soc.* **2021**, *143*, 15924–15929; (c) W. Fan et al., *Nat. Synth*. **2023**, *2*, 880–887; (d) G.-F. Huo et al., *Agnew. Chem. Int. Ed.* **2023**, e20221809; (e) Q. Zhou et al., *Angew. Chem. Int. Ed.* **2023**, *62*, e202302266; (f) G. Huo et al., *Angew. Chem. Int. Ed.* **2024**, e202403149; (g) Q. Zhou et al., *Angew. Chem. Int. Ed.* **2024**, e202417749; (h) G.-F. Huo et al., *Angew. Chem. Int. Ed.* **2024**, *63*, e202416707.

Aggregation-induced thermally activated delayed fluorescence in diindoloquinolinoacrydines

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Thermally activated delayed fluorescence (TADF) materials are central to the development of high-efficiency organic light-emitting diodes (OLEDs), typically relying on charge-transfer (CT) excited states to achieve small singlet–triplet energy gaps (ΔEST) [1]. Here, we report three N-embedded spiro-based emitters (SDIQA1–3) derived from a fused diindoloquinolinoacridine (DIQA) scaffold and investigate their photophysical behaviour in solution and solid-state environments. Steady-state spectroscopy reveals dual emission, with a high-energy band (~400 nm) assigned to isolated molecules and a lower-energy band (~530–590 nm) emerging in chloroform solution and PMMA films. Excitation-dependent measurements confirm that the red-shifted emission originates from aggregated species. Time-resolved spectroscopy demonstrates microsecond delayed fluorescence exclusively from the aggregate state, while the isolated molecules exhibit only prompt fluorescence and low-temperature phosphorescence. The delayed component shows linear laser power dependence and clear thermal activation, confirming a unimolecular TADF mechanism and excluding triplet–triplet annihilation. Temperature-dependent measurements further reveal phosphorescence from the non-aggregated species at low temperatures. Notably, TADF arises from aggregated states without involvement of conventional CT excited states, indicating a small singlet–triplet gap intrinsic to the aggregate. These findings establish aggregation-induced TADF in a purely nitrogen-embedded framework and provide new design principles for narrowband, non-CT TADF emitters for optoelectronic applications.

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References
Eli Zysman-Colman et al. Chem. Rev. 124, 13736 (2024)

Ambient Direct Arylation Synthesis of Thienothiophene Based Copolymers with Mixed Alkoxy and Oligoether Side Chains

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Conjugated polymers with both oligoether and alkoxy side chains are an emerging type of organic mixed ionic-electronic conductor. Here, direct arylation polymerization is introduced as a viable synthetic route for such materials. The composition and molecular weight of the synthesized thienothiophene-based random copolymers are determined with high-temperature 1H NMR spectroscopy. Chemical and electrochemical doping of the copolymers reveal that the introduction of a minor fraction of alkoxy side chains results in materials with a highly promising set of electrical and mechanical properties. A copolymer with an alkoxy side chain fraction of 12 % features an electrical conductivity of 390 S cm-1 and a charge-carrier mobility of about 3.2 cm2 V-1 s-1. Organic electrochemical transistors with a NaCl aqueous electrolyte feature a high figure of merit of 1313 F cm−1 V−1 s−1 thanks to a high volumetric capacitance of 417 F cm-3. Evidently, the introduction of a minor fraction of alkoxy side chains is a viable route for improving the electrical properties of organic mixed ionic-electronic conductors.

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References

A. Giovannitti, I. P. Maria, D. Hanifi, M. J. Donahue, D. Bryant, K. J. Barth, B. E. Makdah, A. Savva, D. Moia, M. Zetek, P. R. F. Barnes, O. G. Reid, S. Inal, G. Rumbles, G. G. Malliaras, J. Nelson, J. Rivnay and I. McCulloch, Chem. Mater., 2018, 30, 2945-2953.

N. Siemons, D. Pearce, H. Yu, S. M. Tuladhar, G. S. LeCroy, R. Sheelamanthula, R. K. Hallani, A. Salleo, I. McCulloch, A. Giovannitti, J. M. Frost and J. Nelson, Proc. Natl. Acad. Sci. U. S. A., 2023, 120, e2306272120.

J. Kimpel, Y. Kim, H. Schomaker, D. R. Hinojosa, J. Asatryan, J. Martín, R. Kroon, M. Sommer and C. Müller, Sci. Adv., 2025, 11, eadv8168.

Amplified chiroptical properties of N-Heteropolycycles in the crystalline solid

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Chiral N-heteropolycycles can be readily tailored with respect to their electronic state energies and spatial localization through isosteric nitrogen insertion, notably without significantly perturbing their chiral molecular framework. In this work, we investigate a chiral *N*-substituted perylene diimide (PDI) derivative based on a tetraazaperylene core, namely a BINOL-bridged octaazaperopyrenedioxide (OAPPDO).[1] In solution, the compound exhibits strong luminescence but only weak chiroptical activity ($g_{lum} = 2\times10^{-4}$). Upon thermal annealing, polarized optical microscopy reveals the formation of crystalline spherulitic structures, which were further examined with respect to their (chir)optical properties. Owing to the high racemization barrier of the OAPPDO system, annealing temperatures up to 240°C could be applied without loss of chirality. Importantly, no significant changes are observed in the absorption or emission spectra when comparing non-annealed and annealed films, thereby excluding H- or J-aggregate-type optical behavior. However, both circular dichroism (CD) and circularly polarized luminescence (CPL) increase by approximately two orders of magnitude upon annealing ($g_{lum} = 6\times10^{-2}$). Using a custom-built CPL setup,[2] we further deconvoluted linear polarization contributions to the emission via sample rotation. Additional optical anisotropies were analyzed by Mueller matrix microscopy, providing deeper insight into the origin of the enhanced chiroptical response.[3]

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References

B. Rojas-Deij, L. Schneider, T. Bruckhoff, R. Eichelmann, P. Rohrmann, R. Candalh, J. Ballmann, F. Deschler, and L.H. Gade, Chem. Eur. J. 32, e02906, 2026

M. Miah, J. Zerhoch, P. Kollenz, N. Solhtalab, F. Deschler, manuscript in preparation

L. Schneider, E. Vandevoir, N. Mueller, B. Rojas-Deij, L.H. Gade and F. Deschler, manuscript in preparation

Anti-Kasha fluorescence, ultra-long room-temperature phosphorescence and delayed fluorescence from a nearly flat non-symmetric polycyclic aromatic hydrocarbon

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We introduce monohomotruxene (MHTX), a non-symmetric polycyclic aromatic hydrocarbon (PAH) designed by reducing the symmetry of homotruxene (HTX)[1] and truxene (TX)[2]. This partial planarization greatly enhances the complex photophysics over symmetric, triply twisted HTX, substantially increasing the photoluminescence quantum yield (PLQY) in both solution and solid state, a result we attribute to its enhanced molecular rigidity and symmetry breaking. MHTX displays a dual-fluorescence behaviour, yielding prompt fluorescence from S_1, as well as Anti-kasha emission from S_2. Excitation of the S_2 state under anaerobic conditions produces intense cyan long room-temperature phosphorescence (RTP), lasting over 12 s at room temperature. In contrast, excitation to the S_1 state yields aggregate phosphorescence and weak delayed fluorescence (DF) by triplet-triplet annihilation (TTA), in the neat film. Therefore, S_1->T_n intersystem crossing is neglectable. These findings establish MHTX as a highly promising new emissive scaffold, highlighting the remarkable potential of non-symmetric PAH architectures for accessing complex excited-state dynamics and advanced photophysical functionalities.

References

Salla, C. A. M. et al. Persistent Solid-State Phosphorescence and Delayed Fluorescence at Room Temperature by a Twisted Hydrocarbon. Angew. Chem. Int. Ed. 58, 6982–6986 (2019).

Baunsgaard, D. et al. Vibronic Activity in the Phosphorescence Spectra of Disklike Aromatic Molecules: A Combined Experimental and Theoretical Investigation. J. Phys. Chem. A 102, 10007–10016 (1998).

Bridgehead Annulated Triptycenes with Axial Chirality as Scaffolds for CISS and CPL Enhancement

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The Chiral Induced Spin Selectivity (CISS) effect is a phenomenon where chiral molecules can preferentially transport electrons of one spin orientation. CISS is thought to arise from the interaction between the chiral molecule and the spin of electrons, which can be influenced by the molecular structure and the presence of spin-orbit coupling. Another material application of chiral molecules is the emission of circularly polarised luminescence (CPL) which can be applied to improving the performance of optical materials and quantum computing. Molecular topology greatly influences luminescence efficiency, charge transport, and its processability. Towards understanding CISS and exploiting CPL, new molecular archetypes are therefore required. Here we present the synthesis of axially chiral triptycenes with new rings annulated between the bridgehead and peri- positions of the two fins [1]. We reveal a practical route to the resolution of the two enantiomers using asymmetric transfer hydrogenation (ATH) leading to enantioenriched diketones with ee% of up to 96%. Subsequent addition of anthryl groups has been performed to examine and quantify the chiroptical properties of these new luminophores by introducing active substituents that will help improve the dissymmetry factors through rigidification and electron localisation. Initial insights have been made into the chiroptical properties of the enantioenriched samples using circular dichroism (CD) spectroscopy and optical rotation measurements with the CD spectra revealing typical mirror-image Cotton effects.

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References
Warrington, S.; Reponen, A.-P. M.; Deshpande, T.; Carolan, T.; Dodd, E.; Coles, S.; Anstoter, C.; Feldmann, S.; Wright, I.; Antti-Pekka, †; Reponen, M.; Carolan, T. L.; Dodd, E. M.; Coles, S. J.; Anstöter, C. S.; Wright, I. A. Localising Multiple Spin-Charge States in Bridgehead-to-Peri Annulated Triptycenes. (2025). DOI: 10.26434/chemrxiv-2025-trzcq.

Brominated Triryl Radical Modified with Carbazole Donor as a Chiral Luminescent Material

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Luminescent organic radicals have recently attracted considerable interest as functional emitters for organic electronics, bioimaging, and emerging quantum technologies. In particular, generating circularly polarized luminescence (CPL) from radicals possessing propeller-type chirality remains challenging because efficient emission, high chemical stability, and sufficiently large racemization barriers must be achieved simultaneously. Here we report a family of brominated chiral radicals, CzTTBrM, 2CzTTBrM, and 3CzTTBrM, obtained by introducing carbazole donor units into a TTBrM framework. The donor–acceptor architecture promotes charge-transfer (CT) excited states, leading to red to near-infrared (NIR) emission with remarkably high photoluminescence quantum yields of up to 74% together with excellent photostability. These radicals also exhibit large racemization barriers (ΔG‡(353 K) = 27.9–29.1 kcal mol^{-1}), enabling the isolation of enantiomerically pure compounds at room temperature. The resolved enantiomers display circularly polarized luminescence spanning the 650–800 nm region with BCPL values of 0.76–1.1, nearly an order of magnitude larger than that of the parent TTBrM radical (BCPL = 0.16). Furthermore, incorporation of the radicals into polystyrene microspheres results in whispering gallery mode (WGM) resonances, representing the first demonstration of WGM emission from luminescent radicals. These findings highlight a molecular design strategy that combines spin, chirality, and luminescence within a single radical framework, providing a promising platform for future applications in electroluminescent devices, bioimaging, and quantum photonic systems.

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References
K. Nakamura, K. Matsuda, K. Anraku, K. Yamaoka, T. Matsumoto, F. Ishiwari, W. Ota, E. Fujiwara, T. Sato, Y. Inoue, S. Kushida, Y. Yamamoto, T. Hosokai, K. Albrecht, ChemRxiv 2026. DOI: 10.26434/chemrxiv.10001675/v1

Charge transfer, polarons formation, and clustering of doped P3HT chains unveiled by first principle molecular dynamics

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Enhancing the electrical conductivity of π-conjugated organic semiconductors is essential to meet the demands of organic thermoelectric applications. Controlling chemical doping requires a detailed understanding of the mechanisms of charge-carriers formation and their relation to the supramolecular organization. In this study, we focus on F4TCNQ-doped P3HT as a prototypical p-type organic semiconductor and investigate polymer–dopant interactions by simulations of increasingly complex systems. Upon doping, two possible charge states can form within the P3HT chains, namely ICTs (or polarons) and molecular charge transfer complexes (CTCs), depending on whether the charge exchange is net or partial, respectively [1]. Studying the conditions under which ICTs and CTCs form is fundamental, since only polarons effectively promote the conductivity increase of pristine P3HT. We will present a theoretical study based on DFTB Molecular Dynamics (MD) and static DFT simulations on the P3HT/F4TCNQ system to rationalize the properties of the different charge transfer complexes that can occur upon doping in solution [2]. The results show that in isolated P3HT chains CTCs are the most favoured complexes, whereas ICTs require F4TCNQ to place between the P3HT lateral hexyl chains, unveiling the crucial role of P3HT aggregation in the formation of polarons. The theoretical prediction of the spectroscopic response, combined with experimental data from both solution and solid-state samples of doped P3HT, highlights the potential of vibrational spectroscopy in distinguishing between ICT and CTC species. The spectra—especially in the IRAV region [3]—are indeed strongly modulated by the extent of charge transferred from the polymer to the dopant. These results pave the way for developing refined models, based on Periodic Boundary Conditions (PBC) calculations, to study the more complex problem related to the formation of charge carriers in the crystalline domains of P3HT.

References

D. A. Stanfield, Y. Wu, S. H. Tolbert, B. J. Schwartz. Chem. Mat. 33, 2343-2356 (2021).

K. Hu, S. Doti, L. Brambilla, M. Del Zoppo, C. Castiglioni, G. Zerbi. Molecules 30, 1403 (2025).

C. Saporiti, L. Brambilla, D. Fazzi, C. Castiglioni. J. Phys. Chem. C 128 , 5189-5205 (2024).

Electrochemical modulation of the elastic modulus of anorganic mixed electronic-ionic conductor

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The mechanical mismatch between rigid electronics and soft biological tissues presents a major challenge in the development of bioelectronic devices. Organic mixed ionic-electronic conductors (OMIECs), particularly conjugated polymers with oligoether side chains, offer promising solutions due to their intrinsic softness, mixed conductivity, and biocompatibility. However, their significant volume changes during electrochemical cycling—driven by ion and water ingress during oxidation and subsequent expulsion during reduction—often lead to drastic changes in stiffness, complicating device-tissue mechanical matching across redox states. Here, we investigate the electromechanical response of a thienothiophene-based conjugated polymer, p(g3TT-T2), functionalized with triethylene glycol side chains. Using electrochemical nanoindentation and structural characterization, we find that this polymer exhibits only a modest increase in elastic modulus from ~100 to 200 MPa upon electrochemical oxidation. This unusual mechanical stability is attributed to a reversible increase in π–π stacking that compensates for swelling-induced softening. Our findings demonstrate that it is possible to design OMIEC materials with stable mechanical properties across redox states, opening new possibilities for compliant, tissue-matched bioelectronic interfaces that remain mechanically invariant during operation.

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References

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Energetic and Structural Origins of TTA Singlet-Formation Probability in Anthracene Upconversion Materials

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Triplet–triplet annihilation upconversion (TTA-UC) merges two low-energy photons into a higher-energy one under weak incoherent excitation, making it attractive for solar energy conversion, bioimaging, 3D printing, etc.[1] A key annihilator parameter is the statistical probability factor, f, which quantifies how efficiently an interacting triplet pair produces the emissive singlet state. However, establishing reliable f trends is challenging because reported values depend strongly on the methodology and on accurate determination of UC and PL quantum yields, including corrections for reabsorption and inner-filter effects.[2,3] This impedes the identification of trends and design rules for high-f annihilators. Using a single experimental setup and analysis workflow, we therefore examine a structurally diverse series of anthracene annihilators to determine how molecular energetics and structure govern the f factor. The studied series spans directly aryl-substituted and alkynyl-bridged derivatives with systematically varied steric demand, symmetry, and conformational freedom. The results indicate that f is governed by coupled energetic and structural factors, with the separation between 2xT1 and T2 energies as the key indicator. The compounds closer to this resonance exhibit lower f, consistent with enhanced upper-triplet-mediated loss. Meanwhile, conformational rigidity and steric design determine whether that energetic advantage is preserved, favoring higher f by suppressing nonproductive relaxation.

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References

[1] L. Zeng, L. Huang, J. Han and G. Han, Acc. Chem. Res. 55, 2604 (2022)

[2] V. Gray, A. Dreos, P. Erhart, B. Albinsson, K. Moth-Poulsen and M. Abrahamsson, Phys. Chem. Chem. Phys. 19, 1093 (2017)

[3] L. Naimovičius, E. Radiunas, M. Dapkevičius, P. Bharmoria, K. Moth-Poulsen and K. Kazlauskas, J. Mater. Chem. C 11, 14826 (2023)

Experimental and theoretical study of columnar liquid crystal arrangements of benzoperylene diimide

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The self-organizing properties of special molecular materials named columnar liquid crystals (ColLCs), leading to the formation of π-columnar stacks, places them as key to next-generation organic electronics, including organic light-emitting diodes (OLEDs), and organic photovoltaics (OPVs) [1]. ColLC materials combine several advantageous properties, including long-range self-assembly, visible light absorption, and tunable surface alignment of the column axes. We have combined experimental and theoretical studies on the structural and electronic properties of the self-assembly of a ColLC derived from benzoperylene diimide, called H4. In this talk we focus on the theoretical study, combining atomistic molecular dynamics (MD) and electronic/optical simulations with Time Dependent DFT (TDDFT). Bulk models were produced via a solvent-assisted removal process [2], modeled using with the OPLS-AA force field implemented in the GROMACS package [3]. Based on the self-organization of H4 molecules obtained from MD simulations, electronic and optical properties of different molecular blocks of up to 5 neighbor molecules were evaluated using TDDFT with the ORCA package [3]. This approach allowed us to investigate the electronic transitions related to the UV-Vis absorption spectra of different columnar-group arrangements, and to compare them with experimental results. We find that the profile of the absorption peak at lower energy (~2.65eV) is related to electronic transitions interestingly coming from the arrangement of molecular π-stacks.

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References

J. Eccher, G.C. Faria, H. Bock et al., ACS Appl. Mater. Interfaces 5, 11935 (2013)

R.M.L. Savedra, M.N.B.L. de Morais, M.F. Siqueira J. Mol. Graph. Model. 117, 108279 (2022)

M. Abraham, A. Alekseenko, V. Basov et al., SoftwareX, 19 (2015); E Runge and E.K.U. Gross, Phys. Rev. Lett. 52, 997 (1984); F. Neese, Comput. Mol. Sci. 2, 73 (2012)

Gold-activated p-doping for organic semiconductors

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Chemical doping plays a critical role in tailing the electronic properties of organic semiconductors (OSCs) and improving device performance across a broad range of technologies. Despite several methods for controlled dopant distribution have been explored, creating doping gradients through simple solution processing remains challenging. Here, we report a gold-activated doping strategy where the dopant is activated at gold electrode surfaces, thus locally oxidizing (p-doping) the OSCs [1]. This reaction produces a doping gradient that extends outward from the gold interface, as verified by spectroscopic and electrical characterization. This approach is applicable to OSCs with ionization potentials spanning more than 1.5 eV and achieves conductivity >1900 S cm−1. To demonstrate the impact of this doping method, we used it to modify contact regions in solution-processed organic field-effect transistors, resulting in reduced contact resistance and improved mobility. This simple, scalable approach enables the creation of doping gradients from solution and opens new opportunities for interfacial tuning in organic electronics.

References

T. Liu, et. al., Nature Materials, https://doi.org/10.1038/s41563-026-02547-0

Influence of host properties and molecular organisation on triplet–triplet annihilation upconversion

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The ability to convert low-energy photons (e.g., infrared) into higher-energy photons (e.g., visible) via triplet–triplet annihilation upconversion (TTA-UC) is important for a variety of applications, including solar energy harvesting, optical communication, and biological imaging. TTA-UC is particularly attractive due to its tuneable excitation and emission wavelengths and its operation under low excitation power densities. [1] However, the underlying mechanism of TTA-UC is complex and depends on several key factors, such as molecular diffusion, triplet exciton generation, and energy transfer dynamics. Here, I will present a series of materials designed to deepen the understanding of the TTA-UC mechanism and to optimise its performance. A combination of optical spectroscopy techniques was used to assess how material properties influence upconversion behaviour. In particular, the study evaluates how structural variations in polymer hosts affect molecular diffusion and, consequently, the overall upconversion efficiency. [2] Additionally, molecular diffusion can also be controlled through molecular organisation and intermolecular interactions. I will further present a study examining the influence of liquid crystal phases, demonstrating that these phases enable tunability and control of TTA-UC responses. [3] These results uncover key structure-property relationships that govern TTA-UC efficiency. By elucidating how these factors influence the underlying mechanism, the study offers insights that support the rational design of upconverting systems. Therefore, these findings contribute to the development of more efficient and tuneable materials for solar energy conversion applications.

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References

Bennison, M. J.; Collins, A. R.; Zhang, B.; Evans, R. C. Macromolecules 2021, 54 (12), 5287–5303.

Bennison, M. J.; Collins, A. R.; Gomes Franca, L.; Burgoyne Morris, G. H.; Willis-Fox, N.; Daly, R.; Karlsson, J. K. G.; Charles, B. L.; Evans, R. C. Mater. Adv. 2025, 6 (3), 1089–1096.

Franca, L. G.; dos Santos, P. L.; Pander, P.; Cabral, M. G. B.; Cristiano, R.; Cazati, T.; Monkman, A. P.; Bock, H.; Eccher, ACS Appl. Electron. Mater. 2022, 4 (7), 3486–3494.

Light-responsive structural control in liquid crystals for solar energy storage and beyond

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The sun is the most abundant energy resource on Earth, but effective storage solutions must be found to enable energy supply on-demand. To this end, molecular solar thermal energy storage (MOST) materials are a promising method for renewable energy storage that capture solar energy and release it on-demand as heat.[1] Azobenzene is a photoswitchable molecule that is attractive for MOST applications due to its reversible, E-Z isomerisation. Recently, phase-change materials have been formed using azobenzene to increase its energy-storage capacity; however, these condensed phases often lower the azobenzene isomerisation degree, which is only recovered on dissolution.[2] In this work, sparing solvent addition is used to drive the self-assembly of azobenzene photosurfactants into lyotropic liquid crystal (LLC) phases, which are used here for MOST applications for the first time.[3] Using small-angle x-ray scattering (SAXS) with in-situ differential scanning calorimetry (DSC), isomerisation-induced LLC phase transitions are matched to their energy-storage contributions. Solvent addition both enhances the isomerisation degree (by up to 20%) and amplifies the structural disordering on isomerisation. These combined properties make photoswitchable LLCs an exciting new class of MOST materials, with potential for domestic heating, grid storage, or de-icing applications. In addition, the combination of advanced characterization methods used to establish the structure–isomerization–enthalpy (LLC-photoswitch-phase change) relationships provides unique insight into these multicomponent systems. This information accelerates the design pathways for future iterations of these materials for solar energy storage and beyond, including as targeted drug delivery vehicles and control gates for microfluidic reactions.

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References

Z. Wang, P. Erhart, T. Li, Z-Y. Zhang, D. Sampedro, Z. Hu, H.A. Wegner, O. Brummel, J. Libuda, M.B. Nielsen, K. Moth-Poulsen, Joule, 5, 3116 (2021).

K. Masutani, M. Morikawa, N. Kimizuka, Chem. Commun., 50, 15803 (2014).

B.E. Jones, Z. Wang, M.A. Zwijnenburg, C.J.C. Edwards-Gayle, K. Moth-Poulsen, N. Cowieson, R.C. Evans. J. Am. Chem. Soc., 147, 29349 (2025).

Mixed Micelle Thermodynamics and Interfacial Control in Surfactant-Assisted Sol–Gel Ga2O3 Thin Films

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Control over thin-film morphology in sol–gel dip-coating strongly depends on the self-assembly behavior of surfactant–precursor systems. In this communication, gallium oxide (Ga_2O_3) thin films were prepared using nonionic surfactants (Triton X-100 and Brij L4) and mixed micellar formulations to investigate how micellar thermodynamics influences film formation and densification[1]. Optical transmittance measurements of surfactant solutions reveal progressive attenuation with increasing surfactant concentration, consistent with enhanced Rayleigh scattering from micelles with estimated diameters of approximately 5–10 nm [2]. These results indicate that micelle density and aggregation significantly modify the colloidal structure of the precursor sol. Thermal analysis (TG–DTA) further shows that Brij-rich systems retain up to ~15–17% bound solvent, leading to slower evaporation and modified decomposition pathways during calcination. Atomic force microscopy reveals that films prepared near the critical micelle concentration (CMC) exhibit sparse nucleation sites and isolated surface structures, whereas intermediate surfactant concentrations produce more homogeneous coverage and increased surface roughness. At higher concentrations, larger discrete aggregates reappear, suggesting micelle reorganization during gelification. X-ray diffraction confirms the formation of β-Ga_2O_3 after calcination, with surfactant-assisted samples showing enhanced peak intensity and improved crystallinity compared to surfactant-free systems. These results demonstrate that micellar phase behavior and surfactant composition provide an effective strategy to control precursor organization, nucleation dynamics, and microstructure in sol–gel derived oxide thin films, all of which are of interest in the development of optoelectronics, gas-sensors and photocalyst samples.

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FAPESP process 2022/13479-1

References

U. Černigoj, U. L. Štangar, P. Trebše, U. O. Krašovec and S. Gross, Thin Solid Films 495, 327 (2006)

G. Puača, V. Tepavčević and M. Poša, J. Chem. Thermodyn. 173, 106835 (2022)

Modulating Singlet-Triplet Transitions in Benzofluorene Diradicals via Conformational Locking of Quinoidal/Aromatic Hybrid

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Qubits (quantum bits) are the fundamental units of information for Quantum computing. However, most molecular qubits require extremely low temperatures to work.[1] Conjugated organic diradicals, organic molecules with two slightly coupled unpaired electrons in their open-shell form, have emerged as promising candidates to overcome this limitation.[2] The presence of these two coupled unpaired electrons, enables accesible low to high spin transitions at room temperature. In this work, we present a series of symmetrical Chichibabin's hydrocarbons, namely (CHs), CH(0)-CH(3).[3] Across the series, the dihedral angle between the two molecular fragments is progressively increased. We have studied these compounds with a variety of experimental such as ground state absorbance and emission (with variations in temperature), spectroelectrochemistry and transient absorption, together with quantum chemical calculations. We demonstrate that, by conformationally locking the angle, we are able to fine-tune the electronic coupling between both diradical electrons. This molecular variation is translated into a precise change in their magnetic properties, by modifying the singlet-triplet gap. The locking in the maximal angle shows a deviation born from the complete decoupling between the two radical electrons. This is evidenced by the emissive behaviour of CH(3), a characteristic that is highly unusual for radical species. In addition, given the conjugation breaking, the emission comes from a higher energy state tan S1. Therefore, this work, besides its application in molecular magnetic properties for quantum computation provides a new recipe for emissive diradicals, which are, in addition, anti-Kasha emitters.

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References

Fataftah M.S, Freedman, D.E., Chem. Commun., 54(98), 13773-13781 (2018)

Abe M., Chem. Rev., 113(9), 7011-7088 (2013)

Feng Z. et al, Angew. Chem. Int. Ed., e20964 (2025)

Nanoengineered organic pi-conjugated donor-acceptor-donor trimers particles for photocatalytic H2 evolution

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The intermittent nature of renewable energy sources, such as solar and wind, poses a significant challenge globally. Green hydrogen (H2) emerges as a promising solution for energy storage due to its significantly low carbon emissions. While traditional methods for solar-driven H2 production involve photovoltaic energy harvesting followed by water electrolysis, photocatalytic water splitting offers the advantage of combining both processes in a one-pot alternative. In this process, light (e.g. sunlight) is initially absorbed by the active material to generate charge carriers, followed by charge separation. Separated charges (electron/hole) are then transported to the water/particle interface, triggering the redox reactions of water. In this work, a versatile platform for preparing functional nanoparticles via a soap-free miniemulsification/solvent evaporation method is proposed. Donor-acceptor-donor (D-A-D) π-conjugated organic trimers, synthesized through C-C cross-coupling techniques, serve as the active material. In parallel, Reversible Addition-Fragmentation Chain-Transfer (RAFT) polymerization was used for the preparation of an amphiphilic block copolymer. Nanoparticles of the DAD trimers dispersed in an aqueous phase were prepared via a miniemulsification/solvent evaporation method. The hydrophilic segment of the block copolymer not only ensures the colloidal stability but also allows precise control over surface functionalization, introducing functionality to the final particles such as pH-responsiveness. The resulting aqueous nanoparticle dispersions demonstrate high photocatalytic activity for H2 generation via water splitting, achieving rates exceeding 500 µmol g-1 h-1. These findings pave the way for next-generation photocatalytic H2 production, combining high efficiency with environmentally friendly and safe chemical processes.

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References
T. R. Guimaraes, A. Khan, H. Remita, J. L. Bobet and E. Cloutet. Macromol Rapid Commun, 2024, 45, e2400395.

Organic Electrode Materials with Defined 3D Structures for Multivalent Metal-Ion Batteries

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Organic electrode materials (OEMs) composed of lightweight earth-abundant elements offer promising advantages, including molecular tunability, structural flexibility, and potential compatibility with aqueous systems. Dibenzo[b,i]thianthrene-5,7,12,14-tetraone (DTT) is an OEM which has shown major potential for lithium ion batteries[1][2] and zinc ion batteries[3]. This work investigates how three-dimensional (3D) molecular architectures influence the electronic structure and electrochemical behaviour of DTT-based materials. Dibenzobicyclo[2.2.2]octatriene moieties have been fused onto one or both ends of the thianthrene-5,7,12,14-tetraone core of DTT to form two new thianthrenetetraone OEMs with distinctive 3D structures. These bulky groups mitigate π–π stacking and generate intrinsic porosity to facilitate charge-carrier mobility, and hence improve discharge kinetics, ideally with limited impact on active-group density per unit volume. Using X-ray crystallography in conjunction with computational approached, we identify that there is a surprising amount of flexibility across the central sulfur-sulfur axis of the molecule. The optical and electrochemical properties are reported in solution and thin film alongside aspects of the relative performance of these molecules in aqueous zinc ion batteries. These results demonstrate that increasing the 3D character through the triptycene motif can modulate reduction potentials and intermolecular interactions without dramatically changing the electronic structure and electrochemical behaviour.

References

[1]T. Ma, Q. Zhao, J. Wang, Z. Pan and J. Chen, Angew. Chem. Int. Ed., 55, 6428–6432 (2016).

[2] X. Deng, L. Liu, S. Zhang, Q. Chen, X. Zhang, H. Wu, Y. Chen, T. Hou, M. Liu, D. Zhou, L. Peng and Z. Chen, Nat. Chem., 17, 1546–1555 (2025).

[3]Y. Wang, C. Wang, Z. Ni, Y. Gu, B. Wang, Z. Guo, Z. Wang, D. Bin, J. Ma and Y. Wang, Adv. Mater., 32, 2000338 (2020).

Red-emitting dimethoxy/difluorobenzothiadiazoles core materials for OLED with stable warm-white electroluminescence

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References
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Room temperature Coulomb gap signatures in PEDOT

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The thermoelectric figure of merit ZT = $S^2\sigma T/\kappa$ (or correlatively, power factor PF = $S^2\sigma$) in organic semiconductors remains fundamentally constrained by the strong interdependence of electrical conductivity σ and Seebeck coefficient S. π-conjugated polymers are eminently promising organic materials, achieving PF values up to ~1.3 mW m-1 K-1 [1]. Our previous work [2] introduced a novel strategy to enhance PF of IDTBT by simultaneously increasing σ via doping and boosting S through a soft Coulomb gap near the Fermi level. A nonlinear drain-current feature in field-effect (FE) characteristics, attributed to the Coulomb gap, enabled Seebeck enhancement at an already highly doped state, but was present only at sub-ambient temperatures (<240 K). Here, we report the first room-temperature signatures of a Coulomb gap in the π-conjugated conducting polymer PEDOT, a system in which Coulomb interactions have generally been assumed negligible due to its high carrier density and metallicity. We probe the evolution of the characteristic nonlinear transport feature under controlled variations in temperature, OECT-based ionic doping, microstructural order, and long-term FE biasing. Our findings link electronic transport, ionic relaxation dynamics, and structural order to the emergence and modulation of interaction-induced density of states suppression. These results provide insight into why Coulomb-gap signatures appear only in certain systems and temperature regimes, and how they can be engineered. This work establishes that interaction-induced DOS suppression can persist in metallic π-conjugated polymers at room temperature, providing clear design rules for Coulomb-gap engineering as a pathway toward enhanced thermoelectric performance in practical devices.

References

M. Du et al., Adv. Funct. Mater., 35, 1 (2025)

D. H. L. Tjhe et al., Nat. Mater., 23, 12 (2024)

Sequence-defined Pi-conjugated Oligomers for Organic Electronic Devices

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Pi-conjugated polymers represent a unique class of chemical compound that possess exceptional optical and electronic properties which have enabled their rapid implementation in a multitude of organic electronic device applications. These outstanding optoelectronic properties are a result of pi-electron delocalisation and charge-carrier mobility within the polymeric material and are directly affected by structural variations in chain length and monomer sequencing. Further application now necessitates a more comprehensive understanding of the structure-property relationship within these materials and how this can affect device performance. Conjugated oligomers have emerged as an attractive alternative that can effectively probe this relationship. Where traditional polymerisation methods cannot easily control chain length, precise monomer sequencing and monodispersity; the stepwise addition of monomer units to form conjugated oligomers allows for full control over these factors. This works focusses on the optimisation of pi-conjugated oligomer formation, implementing both traditional cross-coupling chemistry and modern purification procedures to facilitate their synthesis. These reactions have been performed using carefully designed monomeric building blocks such that sequential couplings can produce well-defined conjugated oligomers in high yields to allow for more flexibility in the structural design of conjugated materials, alongside producing an innovative and more accessible synthetic route towards their formation.

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Spectroscopic ellipsometry characterization of thin films for application in OPVs

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The morphology of the layers of organic solar cells, such as polymer orientation, cristallinity, domain size in the active layer, and rugosity of interfaces play a key role in the device performance [1]. These parameters are strongly affected by the film deposition technique. In this work we use spectroscopic ellipsometry, a fast and non-destructive technique based on the measurement of the change in the state of polarization of light when it is reflected from the sample, to characterize cristallinity, rugosity and polymer molecular orientation in thin films of materials for organic photovoltaics. The orientation of polymer chains can be obtained by modeling the material as an uniaxial anisotropic material and observing the variation between the ordinary and extraordinary refractive indexes. Changes in molecular orientation in Y6:PM6 films due to substrate selection (glass or zinc oxide nanoparticles) were observed for spin coated films. Changes in the film morphology and orientation due to aging were analyzed for a period of 170 days, showing that, in the case of the glass substrate the film changed from edge on orientation to face on orientation [2]. During the experiment modifications in cristallinity were also observed by analyzing variations in the ratio between 0-0 and 0-1 vibronic transitions. The effects of the deposition technique (blade coating or spin coating) in the morphology and orientation of an zinc oxide nanoparticles film, which are anisotropic due to ZnO wurtzite structure [3], were observed. The effects of deposition parameters in the blade coater and the used blade were also analyzed.

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References

Liang, Qiuju, et al. Chemical Engineering Journal, 488, 150783 (2024)

A. Kamptner, M. C. Scharber and M. Schiek, ChemPhysChem, 25, e202400233 (2024)

M.-I. Kang, S. W. Kim, Y.-G. Kim and J. W. Ryu, Journal of the Korean Physical Society, 57, 389–394 (2010)

Spectroscopy to Unravel Symmetry Breaking Structure-Property Relationships aimed at Two-Photon Absorption for Cell Imaging

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Two-photon absorption (2PA) has become an essential tool in bioimaging, highly regarded for its ability to facilitate deep tissue imaging while minimizing photodamage. While several factors influence the 2PA efficiency of a dye, recent studies have uncovered a strong link between 2PA and excited state symmetry breaking (ES-SB).[1] In this work, we investigate a series of molecules exhibiting 2PA, featuring two distinct structural motifs: a dicationic bisindolium series that displays an unusual blue-shifted emission,[2] and a molecule inspired by [n]CPP (cycloparaphenylene).[3] These families were characterised using a wide set of spectroscopic techniques, including low-temperature absorbance and emission, two-photon absorbance and emission, and transient absorption spectroscopy. The experimental data, supported with theoretical calculations, provided important insight into the structural origins of symmetry breaking and its implications for 2PA. Furthermore, our approach revealed the mechanism behind the counterintuitive blue-shift emission for the bisindolium familiy. Moreover, these molecules were used for specific mitochondrial staining in living HeLa cells, achieving performance comparable to more complex commercial mitochondrial markers. In summary, this work provides valuable guidelines for the rational design of efficient 2PA emitters tailored for biological imaging applications.

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References

A. Cesaretti, A. Spalletti, et al., Phys. Chem. Chem. Phys., 23, 16739, (2021).

C. Benitez-Martin, J. M. Marin-Beloqui, et al., Adv. Mater., e10730, (2025).

R. Jasti, C. R. Bertozzi, Chem. Phys. Lett., 494, 1–3, 1-7, (2010).

Supramolecular control of excited-state pathways in organic emitters: from TADF and RTP to sensing and singlet oxygen generation

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Thermally Activated Delayed Fluorescence (TADF) and Room-Temperature Phosphorescence (RTP) materials have emerged as key mechanisms for efficient triplet harvesting in purely organic emitters. While these properties are often considered intrinsic molecular features, our recent studies demonstrate that supramolecular packing and nanostructuration can play an important role in controlling the excited-state pathways. In this talk, supramolecular organization is introduced as a design parameter for activating, switching, and tuning TADF and RTP in donor–acceptor (D–A) systems. Three complementary strategies are demonstrated. First, we demonstrate Aggregation-Activated TADF (AA-TADF), where specific π–π stacking motifs induce TADF in molecules that are non-emissive as isolated monomers. Second, we report a geometry-locking mechanism in which crystal packing prevents the molecule from accessing non-emissive orthogonal conformations in the excited state, preserving oscillator strength and activating TADF.[1] Third, by modulating molecular rigidity, we achieve reversible switching between TADF and RTP.[2] We further explore the stimuli-responsive nature of these materials, showing multistage mechanofluorochromic behaviour [3], which opens new opportunities for optical sensing. Finally, we exploit nanostructuring to tune triplet lifetimes, enabling singlet oxygen ($^1O_2$) generation for photodynamic therapy (PDT), time-gated bioimaging with enhanced signal-to-noise ratios, and both oxygen and chemical sensing. Overall, these results demonstrate that supramolecular organization provides a powerful strategy to control excited-state photophysical process in organic emitters, enabling the rational design of multifunctional materials for optoelectronics, sensing and biomedical applications.

References

A. Maggiore et al. Phys. Chem. Chem. Phys., 24, 17770 (2022)

A. Maggiore et al. J. Mater. Chem. C,12, 7943 (2024)

A. Maggiore et al. J. Mater. Chem. C, 1313752 (2025)

Synthesis and photophysical properties of benzoyl-peri-xanthenoxanthenes. Intensely fluorescent ketones.

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Polyaromatic hydrocarbons (PAH) are highly prized molecular semiconductors with numerous applications in organoelectronic devices or as chemical and biological sensors. Peri-xanthenoxanthene (PXX) is a poly-heteroaromatic hydrocarbon (PAH), the structure of which can be considered an O-doped antanthrene (AA).[1] Like many PAH compounds, PXX is intensely fluorescent. The heteroatom doping of the structure significantly perturbs the optoelectronic properties (fluorescence quantum yields: PXX 60%, AA 24%) and the chemical reactivity of the polyaromatic structure. In the present study we have developed synthetic methodology for the regioselective preparation of p-substituted benzoyl-PXX derivatives (XBz-PXX) and characterized their solution photophysical properties. The compounds are bright orange to red colored solids and solutions of the compounds revealed fluorosolvatochromic behavior. The solution UV-vis spectra present a broad absorption band with large molar absorptivity over the range 400 – 530 nm. The absorption onset varies in a systematic and predictable form with the nature of the substituted benzoyl group. Emission spectra of the solutions of XBz-PXX were obtained in solvents of different polarities. In hydrocarbon solvents the emission is vibrationally structured, whilst in polar solvents a broad gaussian type band is observed. The maximum emission wavelength varied with the nature of the solvent (520 to 580 nm). The emission quantum yield (generally between 50 and 70%) was found to be exceptionally large for a benzoyl-PAH structure and lifetimes were typical of fluorescence deactivation (5 ns).[2],[3] The Lippert-Mataga polarizability function was used to analyze the fluorosolvatochromic effect and calculate the difference between molecular ground and excited state dipole moments. TD-DFT calculations were employed to investigate the nature of the electronic transition and the resulting changes to the structure.

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References

D. Zanetti, C. De Luca et al. Nat. Chem. 17, 1138 (2025)

S. K. Rajagopal, K. Nagaraj et al. Phys. Chem. Chem. Phys. 20, 19120 (2018)

Y.Bo, H.Zhang, et al. Angew. Chem. Int. Ed. 63, e202313936 (2024)

Synthesis engineering and development of emergent conducting pi-conjugated materials: applications in energy harvesting and storage devices

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The synthesis engineering and development of poly(3,4-ethylenedioxythiophene):poly(styrenesulfonate) (PEDOT:PSS) have revolutionized the field of conducting p-conjugated materials, offering a robust and versatile platform for energy harvesting and storage applications. By fine-tuning synthesis parameters and doping strategies, the optoelectronic properties of PEDOT:PSS can be tailored for specific optoelectronic applications. Here, we report on recent advancements in the synthesis engineering of PEDOT:PSS inks, specially developed for energy harvesting and storage devices. Of particular interest is the application of the synthesized PEDOT:PSS inks as p-type organic thermoelectric materials, holetransport layers (HTLs) in organic solar cells (OSCs), and battery/supercapacitor electrodes. The PEDOT:PSS inks synthesized herein, based on the Louwet route, were compared with state-of-the-art commercially available PEDOT:PSS inks, demonstrating similar or superior performances. For thermoelectric generators (TEGs), our best formulation exhibited a Seebeck coefficient of approximately 12.6 mV K□1, surpassing the 12.3 mV K□1 of the commercial PEDOT:PSS ink (Cleviost PH 1000). In OSCs, our HTL proprietary ink achieved efficiencies and photovoltaic parameters comparable to those of the well-known commercial Cleviost P VP AI 4083. Similar results were obtained in energy storage devices, where the conductive PEDOT:PSS synthesized herein outperformed commercially available formulations, both in open-circuit voltage and in discharge tests. The insights presented in this manuscript underscore the critical role of fine-tuning and synthesis engineering in advancing high-performance and scalable energy harvesting and storage devices.1

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References

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Tetrameric Architecture of Non-fullerene Acceptors for Improved Morphology and Stable Organic Solar Cells

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Among the various non-fullerene acceptors (NFAs), perylene diimide (PDI) stands out for its large, planar π-surface, good charge transport properties, and absorption in the visible spectrum. However, the highly planar structure of PDI units leads to intense π-π stacking interactions, resulting in strong aggregation and crystallisation in the active layer of organic photovoltaic cells (OPVs), which hinders exciton dissociation. In addition, molecular diffusion of small acceptors further lowers the device efficiency. To address these challenges, we designed and synthesized a tetrameric PDI architecture based on a flexible pentaerythritol core , employing a straightforward and readily accessible synthetic route. This strategy enhances solubility and spatial geometry, making thin films more homogeneous [1]. The properties of the PDI tetramer were compared with its corresponding monomer synthesized in a similar way. The tetramer showed stronger absorbance (εmax = 126,000 M-1 cm-1) than the monomer. Thermal analysis revealed a less crystalline nature for the tetramer relative to the monomer, along with a significant increase in the glass transition temperature (Tg), resulting in lower diffusion coefficient [2,3]. This is crucial for achieving reduced domain sizes and stable active layer morphology with satisfactory OPV performance. Photovoltaic performance was evaluated in OPV devices fabricated from blends of PDI acceptors with a complementary donor polymer. Overall, this synthesis approach highlights the potential of high molecular weight acceptors for efficient NFA-based OPVs.

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References
Labrunie, A.; Josse, P.; Dabos-Seignon, S.; Blanchard, P.; Cabanetos, C. Sustainable Energy Fuels, 2017, 1 (9), 1921–1927.

Wu, L.; Pan, T.; Wang, X.; Hai, Y.; Liu, S.; Ma, R.; Lu, J.; Xiong, L.; Chan, Y.; Dong, J.; Li, Y.; Luo, Y.; Zhu, L.; Xiao, B.; Zhang, J.; Chen, J.; Zhang, T.; Wu, J.; Liu, S.; Jia, T.; Huang, F. Angewandte Chemie International Edition 2025, 64 (36), e202506445.

Ghasemi, M.; Balar, N.; Peng, Z.; Hu, H.; Qin, Y.; Kim, T.; Rech, J. J.; Bidwell, M.; Mask, W.; McCulloch, I.; You, W.; Amassian, A.; Risko, C.; O'Connor, B. T.; Ade, H. Nat. Mater. 2021,

20 (4), 525–532.

The place of iridium complexes on the phosphorescence - TADF spectrum: *Evidence for thermally activated delayed fluorescence in iridium(III) complexes*

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Iridium(III) complexes play a pivotal role in research and technology. They are used in a plethora of applications, from organic light-emitting diodes (OLEDs) and light-emitting electrochemical cells (LEECs), to bioimaging, phototherapy, photochemistry and photocatalysis. The popularity of Ir(III) complexes in OLEDs remains somewhat uncontested, despite the low earth abundance of this metal and enthusiastic efforts to identify alternatives. Although they are widespread, have we really understood fully the excited-state properties of Ir(III) complexes? Our interest in iridium(III) complexes follows our recent works on the subject [1], [2], [3]. In this work we report the second ever example of a fully experimentally confirmed thermally activated delayed fluorescence (TADF) in a dinuclear Ir(III) complex. The said complex displays a singlet-triplet gap ΔEST = 28 ± 5 meV, in agreement with the computational prediction of 31.1 meV. We also demonstrate a proof-of-concept solution-processed OLED featuring this complex as the luminescent dopant in the emissive layer, achieving external quantum efficiency of up to ~10% and maximum luminance of 18 000 cd m-2. These findings are complemented by a detailed consideration of spectral signs of TADF in the already known Ir(III) complexes. In this study, we have scrutinized literature data on iridium(III) complexes that likewise show significant overlap between absorption and PL, and we conclude that a small singlet-triplet energy gap ΔEST in these complexes results in a TADF contribution to their emission. Such a mechanism has hitherto been overlooked in the large body of iridium(III) chemistry. We use computations to clarify the nature of the excited states in these complexes, demonstrating that the distinctive S1 and T1 character of states can be identified as well as confirming that ΔEST is small enough for TADF to occur at room temperature.

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References

[1] Inorg. Chem. Front. 2026; DOI:10.1039/D5QI01968K

[2] Chem. Sci., 2023, 14, 13934–13943; DOI:10.1039/D3SC04450E

[3] Chem. Sci., 2021, 12, 6172–6180; DOI:10.1039/D1SC00160D

The transition between direct and inverted singlet-triplet gaps in nitrogen-substituted phenalene molecules

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Molecules exhibiting inverted singlet–triplet energy gaps challenge Hund's rule and have recently attracted growing interest due to their potential in organic optoelectronic applications, particularly organic light-emitting diodes. In this work, we explore the origin of singlet–triplet inversion in a series of nitrogen-substituted phenalene derivatives. High-level excited-state calculations based on equation-of-motion coupled-cluster theory with single and double excitations (EOM-CCSD) reveal systematic trends associated with chemical substitution and molecular topology, allowing us to identify distinct classes of spin-gap behavior. To gain further insight, we introduce a simple effective model that captures the key electronic features governing these trends. By combining this model with ab initio results, we establish qualitative relationships between molecular structure and spin-state ordering. These findings provide a coherent framework for understanding singlet–triplet inversion in organic systems and offer useful guidelines for the design of new functional molecules.

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References

Dreuw, A.; Hoffmann, M. The inverted singlet–triplet gap: a vanishing myth? Frontiers in Chemistry 2023, 11, 1239604.505

de Silva, P. Inverted singlet–triplet gaps and their relevance to thermally activated delayed fluorescence. The Journal of Physical Chemistry Letters 2019, 10, 5674–5679.510

Wilson, K. D.; Styers, W. H.; Wood, S. A.; Woods, R. C.; McMahon, R. J.; Liu, Z.; Yang, Y.; Garand, E. Spectroscopic quantification of the inverted singlet–triplet gap in pentaazaphenalene. Journal of the American Chemical Society 2024, 146, 15688–15692

Thickness-Dependent Molecular Orientation in Organic Layers: Insights from Single-Molecule Microscopy on Ensemble Trends

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The orientation of organic molecules critically controls the electrical and optical performance of organic light-emitting diodes (OLEDs). Horizontal alignment of emitter molecules can boost light outcoupling by ~50%,1 while the orientation of host and transport-layer materials further modulates outcoupling, charge injection, and transport.2 Despite extensive work, a comprehensive understanding of orientation in thermally evaporated films remains lacking, and conclusions are hard to draw from cross-comparisons across the many different existing studies. Here we present a systematic investigation of molecular orientation in vacuum-deposited host materials and host–emitter systems as a function of film thickness and vertical position. Variable-angle spectroscopic ellipsometry reveals that anisotropic host molecules adopt progressively more horizontal average orientations in thicker films, an effect amplified in birefringent materials. Angle-resolved photoluminescence of host-guest systems shows that host alignment templates the orientation of a small-molecule emitter. We further show that film thickness can dominate over the host glass-transition temperature as a predictor of emitter alignment. Finally, we apply single-molecule orientation and position imaging to map z-dependent emitter orientation distributions,3 revealing interface-driven alignment gradients invisible to ensemble averages. These complementary ensemble and single-molecule results demonstrate that molecular orientation can be strongly influenced by the film interfaces. Crucially, our results indicate that films thinner than ~20 nm—a thickness range frequently used in emitter orientation studies—can yield molecular orientation distributions that differ from bulk films. We conclude with practical fabrication and characterization guidelines to improve accuracy, reproducibility, and cross-comparability in molecular orientation studies for organic semiconductor materials research.

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References

F. Tenopala-Carmona et al., Advanced Materials, 33, 2100677, (2021)

A. Hoffman et al., Advanced Optical Materials, 9, 2101004, (2021)

F. Tenopala-Carmona et al., Nature Communications, 14, 6126 (2023)

Tracking excited-state proton transfer in aromatic compounds

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Proton transfer is one of the most fundamental processes in nature, playing an important role in chemistry, biology, and materials science, from nucleic acids and enzymatic reactions to functional dyes and photoactive materials. Despite extensive theoretical research, direct structural insight into excited-state proton transfer (ESIPT) in the crystalline phase remains limited. I will present results of combined theoretical and experimental studies of two ESIPT-active molecular families: 2′-hydroxychalcones and thiazolo[5,4-d]thiazoles. Theoretical investigations were performed at the TDDFT and NEVPT2 levels to characterize excited-state potential energy surfaces and proton-transfer pathways, with emphasis on the interplay between locally excited and charge-transfer states. The calculated ESIPT energy barriers range from 3 to 20 kcal/mol, corresponding to timescales from sub-femtoseconds to milliseconds at room temperature. Experimentally, single-crystal X-ray diffraction data were refined using the Hirshfeld Atom Refinement (HAR) method [1], enabling accurate determination of hydrogen-atom positions and detailed analysis of hydrogen-bond geometries. These studies were complemented by time-resolved fluorescence measurements probing the dynamics of emissive excited states associated with ESIPT. Correlations were identified between O–H bond lengths in the ground and excited states and the energy barriers. These bond lengths also correlate with fluorescence quantum yields in solution and in the solid state. The combined use of high-level quantum-chemical calculations, advanced crystallographic refinement, and time-resolved spectroscopy provides a strategy for investigating proton transfer directly in the solid state. The results offer new insight into structure-property relationships governing excited-state proton dynamics and lay the foundation for future photocrystallographic studies aimed at direct observation of proton motion in crystals.

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References
Capelli, S. C., Burgi, H.-B., Dittrich, B., Grabowsky, S. & Jayatilaka, D. (2014). IUCrJ, 1, 361-379.

Tuning Optoelectronic Properties of Organic Semiconductors through Boron-Nitrogen moieties

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The introduction of boron-nitrogen (B-N) moieties in pi-conjugated systems represents a promising tool for developing high-performance and stable organic photovoltaic cells (OPVs). These motifs can be classified according to the nature of their interaction, namely B←N coordinate bonds and a B–N covalent bonds. The first one exhibits a stronger electron withdrawing character and larger dipole moment, which translates into a red-shifted absorption and modified packing behavior.[1] The second is associated with singlet-triplet energy gap suppression, leading to reduced non radiative recombination losses.[2] Thus, incorporating these B-N units into π-conjugated frameworks improves the optoelectronic properties of organic semiconductors and corresponding OPVs. In our contribution to the field, a series of B-N doped polycyclic aromatic hydrocarbons have been designed and synthesized, exploring both B←N motifs (BNBP and BOIMPY) and covalent B-N units, including a novel structure resembling the Y6 backbone. Their optical properties have shown sharp absorption spectra extending, for some compounds, into the near-infrared region. Furthermore, their molecular structures exhibit high coplanarity, promoting ordered molecular packing. To assess the compatibility of these materials as non-fullerene acceptors (NFAs) in OPVs, we have studied their processability through vacuum and solution-processed techniques. For a BNBP-based compound, evaporated thin films have been prepared for the first time, yielding good absorption properties. As for the BOIMPY derivatives and new covalent B-N based compounds, structural modifications are being implemented through molecular chain engineering to enable their compatibility with solution-processed fabrication techniques. Given their morphological and optical advantages, these materials show great potential in both vacuum-deposited and solution-processable OPVs.

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References

Shao X, Liu M, Liu J, Wang L. A. Angew Chem Int Ed. 61(34):e202205893. (2022)

Liu X, Pang S, Zeng L, et al. Chem Commun. 58(62):8686-8689. (2022)

Ultrafast Photoconversion Drives Fluorescence Switching in anthracene-functionalized β-diketones

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β-Diketones functionalized with an anthracene unit integrate the photophysical properties of the π-conjugated anthracene core with the coordination features of the β-diketone framework, making them promising for photoresponsive and light-emitting applications [1,2]. Herein, we report the structural and photophysical properties on two newly designed aliphatic (L1) and cyclic (L2) β-diketone molecules containing anthracene chromophore as substitute group, as well as their tris-lanthanum(III) complexes, La(L1)3 and La(L2)3. The organic molecules and complexes were synthetized and characterized by Single-Crystal XRD, High-Resolution Mass Spectrometry and NMR (1H and 13C). Photophysical properties were investigated using steady-state and time-resolved photoluminescence (TRPL) in both solid state (neat, Zeonex, and PMMA-doped films) and solution, at room temperature and 80 K. Density functional theory (DFT) and time-dependent DFT (TD-DFT) calculations were performed to support the experimental results. The aliphatic ligand L1 shows intense green emission (545 nm, ~200 ps) in neat films and in 2-MeTHF solution (10 µM), whereas the cyclic analogue L2 displays weaker emission (495 nm, ~5 ns). Upon UV excitation (355 nm), L1 undergoes rapid photoconversion from green (545 nm) to blue emission (460 nm), as confirmed by femtosecond transient absorption (fsTA), time-correlated single photon counting (TCSPC), and nanosecond TRPL measurements. The sodium salts ($L1-Na^{+}$ and $L2-Na^{+}$) and the corresponding La^{3+} complexes exhibit similar blue emission at 460 nm, indicating that the emitting species originates from an excited-state intramolecular proton transfer (ESIPT) process that stabilizes the keto form. These results demonstrate that anthracene acts as an effective fluorescence probe, dominating emission in the keto state, and highlight the potential of these systems for photoresponsive and luminescent materials.

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References

X.Li, X.Li, S.-Y.Yang, et al., Adv. Optical Mater.13, 30 (2025).

Zhao, Di, et al., Coord. Chem. Rev. 540, 216770 (2025).

Understanding phodecomposition and controlling the singly occupied molecular orbital of polychlorinated triarylmethyl radicals

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Luminescent radicals, the majority of which are derivatives of tris(trichlorophenyl)methyl (TTM), are of significant recent interest because of the unique quantum properties of the doublet excited state. Control of the energy level of the singly-occupied molecular orbital (SOMO) is essential for the design and application of open-shell materials, but most triarylmethyl radicals are very electron-poor and exhibit similar SOMO values. In this work, we show how a combination of chlorine and methoxy substituents in triarylmethyl radicals allows tuning of their SOMO level over a extraordinarily wide range of –5.7 to –3.9 eV. We determine that one-electron oxidation in air limits the SOMO ≤ -4.5 eV to maintain bench stability. Two new stable radicals are characterized by X-ray crystallography, cyclic voltammetry, and luminescence measurements in solution and doped films. Though they show high chemical stability, most trityl radicals show very poor photostability, which hinders their application as magnetic, optical and quantum-related materials. We use density functional theory to study the mechanism of photodegradation of TTM. We isolate the photodecomposition products and characterize them via mass spectrometry, NMR, EPR, UV-Vis absorption spectroscopy, cyclic voltammetry (CV), and X-ray crystallography. We show that the reaction proceeds by a 5-electron electrocyclization followed by an unusual 1,8-sigmatropic chloride shift, affording two fluorenyl radicals, which slowly oxidize and hydrolyze to form semiquinone products. We examine the reported photostability of >80 substituted triarylmethyl radicals and demonstrate that other common triarylmethyl radicals, including benchmark luminescent derivatives with the highest photostability, the carbazole appended TTMs, photodecompose through the same cyclization mechanism, and thus the DFT-calculated activation energy of cyclization can be used to guide the design of photostability in new luminescent triarylmethyl radicals.

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References
A. Mizuno, R. Matsuoka, T. Mibu, T. Kusamoto, “Luminescent Radicals” Chem. Rev. 2024, 124, 1034–1121.

H. E. Hackney, C. Ruchlin, E. Stahle, D. F. Perepichka, “Chloromethoxytrityls: Tuning the SOMO Level of Stable Luminescent Radicals” Angewandte Chemie International Edition

2025, 64, e202512411.

H. E. Hackney, C. Y. Legault, H. M. Titi, D. F. Perepichka, “Mechanism of the Photodecomposition of Stable Triarylmethyl Radicals” Angewandte Chemie International Edition n.d., n/a, e26004.

Unlocking Trityl Acceptor Polyradicals

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Open-shell luminescence is an emergent field mostly driven by diversifying the tris(2,4,6-trichlorophenyl) methyl (TTM) family [1]. Many TTM-based monoradicals and some diradicals have been reported, but conjugated polyradicals remain scarce due to limitations in the reported methodology. Only donors units were previously polymerised with TTM, and these molecules have shown peculiar properties due to the interaction between their spins and the extensive conjugation such as efficient NIR emission, spin correlation, and remarkable photostability, making them attractive functional materials [2]. We introduce a novel methodology in which a radical monomer is polymerised with acceptor or donor comonomers via base-free Stille cross-coupling, doubling the scope of the reaction. We thus report the synthesis of the first TTM-acceptor conjugated polyradical, alongside another TTM-donor example. We show that this method preserves the radical centres, while also leading to high molecular weights suitable for device fabrication. Preliminary photophysical findings of novel donor-TTM and acceptor-TTM polymers reveal long-lived luminescence, making them promising candidates for device integration. The conventional synthesis of TTM-based conjugated polyradicals involved two steps: the Suzuki cross-coupling of a diboronate radical precursor monomer with a donor dibromo monomer, followed by post-polymerisation deprotonation and one-electron oxidation to generate the radical centres [3]. This strategy is incompatible with acceptor units due to the harsh basic conditions. Moreover, the deprotonation step is a chemical equilibrium, so ensuring complete radical conversion proves remarkably tedious. Our method elegantly circumvents these issues, while also reducing the synthetic time drastically. This key development unlocks new molecular design choices for harnessing their open-shell properties in future photovoltaics and spintronics applications.

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References

[1] A. Mizuno, et al., Chemical Reviews, 124, 3 (2024).

[2] C.P. Yu, et al., Science Advances, 10, 30 (2024).

[3] P. Murto, et al., Nature Communications, 14, 1 (2023).

π-Extended N-Heterocyclic Carbenes: A Platform for Excited-State Control

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Control over excited-state processes in π-conjugated molecular emitters underpins the development of advanced functional materials, yet most designs remain constrained by fixed relationships between electronic structure and emission pathways. Here, we establish π-extended N-heterocyclic carbenes (NHCs) as a versatile platform for controlling excited-state dynamics across multiple regimes. In carbene–gold(I) acetylide complexes, π-extended NHCs induce an imbalance in oscillator strength between excited states. Although internal conversion to first singlet excited state (S1) occurs, this state is effectively dark, while a higher-lying S2 state remains radiatively allowed, resulting in the first demonstration of anti-Kasha electroluminescence. [1] In carbene–platinum acetylides, this design enables access to distinct singlet- and triplet-derived emissive channels, leading to the first demonstration of switchable electroluminescence from a single emitter. In carbene–metal–amide (CMA) systems, π-extension tunes charge-transfer character and suppresses non-radiative decay, enabling efficient reverse intersystem crossing and bright red to near-infrared electroluminescence resulting in an unprecedented 11% external quantum efficiency (EQE) at 170, 000 nits and operating stability (LT97) of 140 h at 1000 nits. In dipolar CMA architectures, the same design enhances third-order optical nonlinearity, enabling two-photon absorption and two-photon excited delayed fluorescence, revealing strong excited-state coupling. [2] Across these systems, π-extension governs orbital distribution, excited-state spacing, and inter-state coupling, providing a unified handle to modulate reverse intersystem crossing, internal conversion, radiative decay, and nonlinear optical response. These results establish π-extended NHCs as a general platform for manipulating energy flow and excited-state behavior in π-conjugated materials.

Acknowledgements
University of Manchester

References

I. D. Nwosu, D. M. De Clercq, S. L. Powley, et al. Anti-Kasha electroluminescence in carbene-gold-arylacetylide complexes. ChemRxiv. (2026). https://doi.org/10.26434/chemrxiv.15000080/v1

I. D. Nwosu, L. Matasović, T. N. Ramos, et al. Enhanced third-order optical nonlinearity in a dipolar carbene-metal-amide material with two-photon excited delayed fluorescence. Commun. Chem (2026). https://doi.org/10.1038/s42004-026-01928-5

Competing copolymer and terpolymer formation in Suzuki reactions: an experimental and thermodynamic insight.

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The donor−acceptor (D−A) approach, with alternating electron-rich (donor, D) and electron-deficient (acceptor, A) units along the conjugated polymer backbone, is an effective method for controlling the optical properties of conjugated copolymers [1]. One strategy to develop alternative D-A polymers is to synthesize random terpolymers by incorporating a third component (such as an acceptor unit) to form a Donor-Acceptor 1-Donor-Acceptor 2 (D-A1-D-A2) chain. Compared to conventional binary D–A copolymers, random terpolymers have been proven to be an effective alternative for controlling optoelectronic properties, such as energy levels, absorption spectra, and aggregation, by varying the proportion of the Acceptor 2 component. In this work, two conventional D−A copolymers and a random terpolymer D-A1-D-A2 composed of fluorene (D), benzothiadiazole (A1), and thiophene-diketopyrrolopyrrole-thiophene (A2) as a building block have been designed, synthesized, and analyzed in terms of optical properties. The D-A1, D-A2, and D-A1-D-A2 systems were synthesized via Suzuki cross-coupling. The chemical structure of the copolymers and terpolymers was determined by NMR and FTIR. The Suzuki reaction used to form the terpolymer D-A1-D-A2 can also yield copolymers D-A1 and D-A2 under the same reaction conditions. The predominance of the terpolymer over the copolymers, or vice versa, depends, among other factors, on thermodynamic and kinetic aspects. The Gibbs energies of the polymerization reactions of these systems were studied using Density Functional Theory at the M06/6-31G(d,p) level. The results obtained show that the reaction to produce D-A1-D-A2 should also form D-A1 and D-A2. TD-DFT absorption spectra, when compared to the measured spectra, corroborate the results of the thermodynamic calculations. Thus, some of the similarities in the experimental and theoretical spectra can be explained by the mixture formed during terpolymer synthesis.

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References
G. L. Heintges and R. A. J. Janssen. J. Phys. Chem. C 124, 3503 (2020)

Conjugated Polymer-TEMPO Hybrid Electrodes for electrocatalytic Alcohol Oxidation

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Electrosynthesis is a sustainable approach that uses electricity to drive chemical reactions. For example, selective alcohol oxidation to form aldehydes typically requires toxic and carcinogenic chromium-based oxidants. Instead, the reaction can be electrified by oxidizing alcohols at the anode in the presence of electrocatalytic mediators like (2,2,6,6-Tetramethylpiperidin-1-yl)oxyl (TEMPO). Grafting TEMPO onto electrodes showed promising results for heterogeneous catalysis to limit additional separation steps and remove molecular catalysts from the product. Challenges remain for developing TEMPO-based electrode materials with efficient charge transport properties, where conjugated polymers are an interesting class of material to improve the charge transfer processes. In my presentation, I will show how metal-free electrodes based on conjugated polymers enable the selective oxidation of alcohols to aldehydes in the presence of TEMPO. Polymers with identical backbone chemistries but varying side chains were synthesized to tune the local environment of the polymer, enabling rapid electron transfer reactions with TEMPO to selectively oxidize alcohols to aldehydes. These polymers were thoroughly purified by preparative high performance liquid chromatography (HPLC) to ascertain that the observed electrochemical activity exclusively originates from the conjugated copolymer, rather than residual metals introduced during the synthesis.

Acknowledgements
We acknowledge financial support from the VR project 023-04203.

References

Semmelhack, M. F.; et al. J. Am. Chem. Soc. 1983, 105, 4492.

Prudlik, A.; et al. Chem. Eur. J. 2023, 29, e202202730.

Connectivity and torsional control of TADF in Carbazole-Triazine star-shaped emitters

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The efficiency of thermally activated delayed fluorescence (TADF) in donor-acceptor (D-A) molecules is governed by a well-stablished paradox: small spatial overlap between HOMO and LUMO leads to a decrease in the energy gap between S1 and T1 (ΔES1-T1). However, this also causes a reduction of the fluorescence radiative decay rate. To further investigate this, we studied the TADF properties of a series of emitters composed of carbazole and sym-triazine as donor and acceptor moieties, respectively, connected via phenylene bridge. We probed the impact of meta versus para substitution pattern, as well as of methyl substitution of the phenylene linkers, on key TADF parameters, such as ΔES1-T1, the photoluminescence quantum yield (PLQY) and delayed fluorescence lifetime (τDF). We found that the TADF properties change dramatically upon these structural modifications: Due to deteriorated oscillator strength, the PLQY drops sharply when torsion comes very close to orthogonality upon double methyl substitution; only para bridging allows coexistence of delayed fluorescence with room temperature phosphorescence in the solid; the smallest singlet-triplet energy gap (ΔES-T) and the fastest TADF result from methyl-substituted meta-bridges, whereas by far the greatest emission quantum yields are observed upon methyl-substituted para-bridging.

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References
T. Y. Li, et al., J. Mater. Chem. C Mater.,10, 4674 (2022)

Crystalline Host–Guest Geometry Locking for High-Speed RISC in TADF Emitters

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Rapid reverse intersystem crossing (RISC) is essential for suppressing triplet accumulation and mitigating efficiency roll-off in blue thermally activated delayed fluorescence (TADF) OLEDs. Here, we introduce a host-driven strategy to boost RISC by enforcing molecular geometry adaptation of a TADF emitter within a crystalline host. A crystalline isophthalonitrile-based host with a nearly orthogonal donor–acceptor (D–A) architecture was designed to impose a more twisted conformation on the doped blue TADF emitter DMeCz-IPN. Single-crystal X-ray diffraction reveals that the dopant adopts the host's pre-twisted geometry, leading to a pronounced reduction of the singlet–triplet energy gap (ΔE_st). As a result, the RISC activation energy is lowered to 23 meV, yielding an almost tenfold enhancement of the RISC rate to above 1×10^7 s^{-1} and a fourfold shortening of the delayed fluorescence lifetime to 1.5 μs. In addition, the crystalline host suppresses conformational disorder, resulting in a narrower emission bandwidth and improved spectral stability compared to amorphous hosts. This work demonstrates crystalline host–guest geometry locking as an effective route for RISC engineering in TADF systems and highlights its potential for the development of high-performance, stable blue OLEDs.

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References
G. Kreiza, T. Javorskis, E. Orentas, and K. Kazlauskas, Adv. Optical Mater. 12, 2400024 (2024)

Design and Synthesis of Dithienothiophene-Based Donor–Acceptor Conjugated Polymers for Energy Applications

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In this study, two novel donor–acceptor type conjugated polymers, P1 and P2, based on dithienothiophene (DTT) building blocks were successfully synthesized via Stille cross-coupling polymerization. The molecular design integrates electron-rich DTT cores with thiophene or 3,4-ethylenedioxythiophene (EDOT) donor units and electron-deficient benzotriazole (BTZ) acceptor moieties to construct a highly planar and extended π-conjugated backbone. The incorporation of cyano-functionalized phenyl substituents further modulates the electronic structure and enhances intermolecular interactions. The synthesized polymers were fully characterized by NMR, GPC, FT-IR, UV–Vis absorption, fluorescence spectroscopy, cyclic voltammetry, TGA, and DSC analyses. Optical measurements revealed broad absorption profiles and reduced optical band gaps, indicating effective intramolecular charge transfer (ICT) within the D–A framework. Electrochemical studies demonstrated tunable HOMO–LUMO energy levels, suitable for energy storage and optoelectronic applications. To enhance electrochemical performance, P1 and P2 were non-covalently hybridized with single-walled and multi-walled carbon nanotubes (SWCNTs and MWCNTs). The resulting hybrid materials exhibited improved charge transport properties due to π–π interactions between the conjugated polymer backbone and carbon nanotube surfaces. Preliminary supercapacitor investigations suggest enhanced capacitance and cycling stability compared to pristine polymer films. These findings demonstrate that rational molecular engineering of DTT-based conjugated polymers provides promising materials for next-generation energy storage systems and advanced optoelectronic devices.

References

Strakova, K.; Assies, L.; Goujon, A.; Piazzolla, F.; Humeniuk, H. V.; Matile, S. Dithienothiophenes at Work: Access to Mechanosensitive Fluorescent Probes, Chalcogen-Bonding Catalysis, and Beyond. Chemical Reviews, 2019, 119, 10977–11005. DOI: 10.1021/acs.chemrev.9b00279

Bronstein, H.; Chen, Z.; Ashraf, R. S.; Zhang, W.; Du, J.; Durrant, J. R.; et al. Thieno[3,2-b]thiophene–Diketopyrrolopyrrole-Containing Polymers for High-Performance Organic Field-Effect Transistors and Organic Photovoltaic Devices. Journal of the American Chemical Society, 2011, 133, 3272–3275. DOI: 10.1021/ja110619k

Şahin, Esra; İşçi, R.; Dönmez, K. B.; Çobandede, Z.; Eroğlu, M. S.; Öztürk, T. Thienothiophene and single-wall carbon nanotube-based hybrid materials: design, photophysical properties and the construction of high-performance supercapacitors. Journal

of Materials Chemistry C, 2025, 13, 17933–17948. DOI:

Diphenyl sulphone core carbazole dendrimers for blue light-emitting electrochemical cells

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Light-emitting electrochemical cells (LEC) are solution-processable solid-state lighting. In our previous work, we have demonstrated that a yellow LEC device with triphenyl-triazine core and methoxylated carbazole dendrimer exhibit a device lifetime of more than 1000 hours. In this study, we focused on blue LEC devices. Blue LECs generally have poor durability. The lack of high-efficiency materials needs to be solved, and hence, the development of new materials is required. Donor-acceptor type dendrimers with diphenyl sulfone core (acceptor) and methyl-substituted carbazole dendron (donor) were developed. Blue LECs were successfully obtained. The photoluminescence studies have indicated the dual emission of fluorescence and room temperature phosphorescence.

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References
L. M. Cavinato, K. Yamaoka, S. Lipinski, V. Calvi, D. Wehenkel, R. van Rijn, K. Albrecht, R. D. Costa, Adv. Funct. Mater. 2023, 33, 2302483.

Dyads Derived from 3,5-Dimethylphenol and 1,8-Naphthalimide: Synthesis, Characterization, and Applications

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1,8-Naphthalimide derivatives are widely investigated due to their favourable photophysical properties and broad applications in sensing, biomedicine, and organic electronics [1]. In organic photovoltaics, they function as electron acceptors, improving charge separation and thermal stability; however, limitations such as low efficiency, poor donor miscibility, and difficulties in thin-film formation persist [2]. In this work, donor–acceptor (D–A) systems based on *1,8-naphthalimide* functionalized with *3,5-Dimethylphenol*-derivatives units were developed to modulate electronic properties, reduce the band gap, and extend light absorption. Three dyads were synthesized, consisting of *1,8-naphthalimide* linked to (*i*) *3,5-Dimethylphenol* via a two-carbon spacer (NEX), (*ii*) *3,5-Dimethylphenol* via a six-carbon spacer (NHX), and (*iii*) *4-hydroxy-3,5-dimethylbenzonitrile* via a six-carbon spacer (NEX-CN). The compounds were characterized, and their photophysical, electrochemical, and morphological properties were evaluated, along with their performance in organic photovoltaic devices. The results demonstrate that structural modifications strongly influence material properties. NEX-CN exhibited a bathochromic shift and more favourable reduction potential, indicating enhanced electron-withdrawing character. While NHX showed superior film morphology, NEX-CN achieved the best photovoltaic performance, with higher VOC, JSC, power, and efficiency, likely due to improved exciton separation. All dyads outperformed N719 dye in DSSCs, with efficiency gains up to 84%, highlighting molecular design as an effective strategy for optimizing photovoltaic materials.

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References
[1] - S. Kagatikar, et al., Journal of Electronic Materials 52, 5401 (2023).

[2] - J. Zhang, et al., ACS Appl. Mater. Interfaces 8, 5475 (2016).

Effect of Molecular Structure on the Interfacial Organization and Rheology of Langmuir Monolayers

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Liquid crystals are promising materials for device development due to their self-organization, which can be enhanced by incorporating photochromic groups to introduce photoresponsiveness and mesophase control. Understanding their structural conformation and stability during immobilization is essential for improving optoelectronic performance. In this context, Langmuir monolayers provide a useful platform to investigate molecular organization at the air–water interface. In this work, we studied the liquid crystal N'1,N'3-bis[(E)-3,4-bis(dodecyloxy)benzylidene]isophthalohydrazide (HDZ) and a structurally related molecule with additional dodecyloxy chains (3C), which does not exhibit liquid crystalline behavior, to evaluate the effect of phase transitions on monolayer formation. Both compounds showed amphiphilic behavior, forming stable interfacial films. Surface pressure–area isotherms revealed similar compressibility moduli (~210 mN m^{-1} at 20 mN m^{-1}), indicating highly packed monolayers. However, HDZ exhibited expansion, while 3C showed contraction, suggesting stronger cohesive interactions in 3C and restricted lateral aggregation in HDZ. Dilatational rheology experiments revealed clear differences in viscoelastic response. The 3C monolayers exhibited higher viscoelastic moduli, indicating a more rigid yet dissipative film, whereas HDZ presented a lower phase angle, consistent with a more elastic, solid-like response. These results indicate that additional alkyl chains in 3C enhance intermolecular cohesion and mechanical strength but increase energy dissipation, while the liquid crystalline organization of HDZ leads to a more elastic structure with reduced viscous losses. Overall, these findings highlight the influence of molecular structure on interfacial organization and viscoelastic behavior, contributing to the design of functional optoelectronic materials.

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References

de Oliveira, W. A.; Alaasar, M.; Cao, Y.; Westphal, E. 1,4-Bis(Acylhydrazone)-Based Polycatenar Liquid Crystals: Self-Assembly, Molecular Switching, and Gelation Properties. ACS Omega 2025, 10 (21), 21637–21647.

Malakhova, Y. N.; Stupnikov, A. A.; Chekusova, V. P.; Kuznetsov, N. M.; Belousov, S. I. Rheological Behavior of Polydimethylsiloxane Langmuir Layers at the Air-Water Interface. Bionanoscience 2020, 10 (2), 403–408.

Electronic Structure and Spin Coupling in Blatter Radical–Fused Phthalocyanines: A DFT Study

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The 1,2,4-benzotriazin-4-yl (Blatter) radical is a persistent open-shell organic system stable under ambient conditions.[1] Recent synthetic advances have enabled systematic functionalization of this scaffold and its incorporation into extended π-conjugated frameworks.[2] In 2025, we reported the incorporation of a Blatter radical into a phthalocyanine framework, affording a β-fused Blatter radical zinc phthalocyanine.[3] Moderate spin communication exists between the radical unit and the macrocyclic π-system. Herein, we present a density functional theory (DFT) investigation of phthalocyanines bearing fused Blatter radicals. Ground-state multiplicities, frontier molecular orbitals, spin density distribution, aromaticity, and optical absorption properties were examined to elucidate spin–electronic coupling. The calculations reveal a near-degenerate manifold of open-shell spin states and significant spin delocalization across the tetra Blatter radical–phthalocyanine, consistent with electronic communication. Time-dependent DFT predicts low-energy absorptions in the near-infrared region, with intensities strongly dependent on the spin reference state. These findings provide insight into structure–property relationships governing spin–photon interactions in conjugated open-shell chromophores.

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References

Blatter, H. M.; Lukaszewski, H. Tetrahedron Lett. 1968, 9, 2701–2705

Ji, Y.; et al. Mater. Chem. Front. 2020, 4, 3433–3443

Hernández, A.; et al. Chem. – Eur. J. 2026, 32, e03294

From Partly Bridged Triphenylamines to Azatriangulenes

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Heterotriangulenes with central N, B, Si or P atoms are C3-symmetry heteroaromatic molecules, which represent an interest as versatile building blocks toward promising materials for next-generation electronic devices.[1] *N*-Heterotriangulenes (azatriangulenes), which are structurally constrained planar analogs of triphenylamines with different bridges between ortho-position of neighboring benzene rings (–O–, $–CH_2–$, $–CR_2–$, –C(=O)–, $–C(=CR_2)–$, –S–), have been actively investigated in recent years.[1,2] π-Conjugated functionalized derivatives of azatriangulenes have been studied as light-emitting materials in OLEDs, charge-transporting materials, as dyes in dye-sensitized solar cells (DSSCs), in design of covalent organic frameworks (COFs), etc. Partly “cyclized” triphenylaminesa with only two bridges have also been studied, mostly toward light emitting materials (particularly, materials showing thermally activated delayed fluorescence, TADF) for OLEDs.[3]

In this presentation, we report our work on functionalization of triphenylamines toward azatriangulene derivatives and partly bridged triphenylamines, mostly focusing on –S–, $–SO_2–$ and –N– bridges. We will present synthetic routes which we exploited in our design and characterization of target products, as well as preliminary results on their optical (electron absorption and photoluminescence) properties.

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References

[1] M. Hirai, N. Tanaka, M. Sakai, S. Yamaguchi, Chem. Rev. 2019, 119, 8291−8331.

[2] J. Borstelmann, V. Gensch, D. Fehn, M. E. Miehlich, F. Hampel, F. Rominger, K. Meyer, M. Kivala, Angew. Chem. Int. Ed. 2025, 64, e202423802.

[3] J. Haug, S. Wu, H. Hafeez, M. Schustek, M. Fatahi, Y. T. Woordes, M. Nieger, O. Fuhr, B. Luy, I. D. W. Samuel, S. Bräse, E. Zysman-Colman, Adv. Optical Mater. 2025, 13, e02118.

Giant surface potential of vacuum-deposited carbazole dendrimers films with fluorinated substituents

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Spontaneous orientation polarization (SOP) is a phenomenon in which the permanent dipole moment (PDM) of polar organic molecules is partially oriented on the substrate during vacuum deposition. As a result of SOP, a giant surface potential (GSP) proportional to the film thickness is generated at both ends of the film. GSP affects the characteristics of OLED devices. The application of SOP to electret materials for vibration power generation devices is also attracting attention. Increasing the GSP slope (surface potential per film thickness) of electret materials is required to enhance the performance of the vibration power generator. Increasing the PDM and degree of orientation of the molecule is considered as a key to obtaining a large GSP slope. Functional groups, such as phosphine oxide[1] and fluorine[2], are effective in controlling molecular orientation. However, the SOP behavior is based on a complex mechanism and is not yet fully understood. In this study, we focused on carbazole dendrimers due to the relatively large PDM, high glass transition temperature, and stable conformation. In particular, we investigated the effect of molecular structure on GSP and SOP by vacuum depositing dendrimers with fluorinated substituents. All dendrimers were oriented so that the outer layer faces the substrate (film), and the more fluorinated substituents in the inner layer of the dendrimers resulted in the larger GSP.

Acknowledgements
JKA Social Action

References

W. Brütting, A. Cakaj, M. Schmid, A. Hofmann, ACS Appl. Mater. Interfaces, 15, 54721 (2023).

M. Tanaka, H. Nakanotani, C. Adachi, M. Auffray, Nat. Mater., 21, 819 (2022).

High-Performance Organic Mixed Ionic-Electronic Conductors Enabled by Thienoisoindigo-Based Polymers

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Organic electrochemical transistors (OECTs) are a key technology in bioelectronics, enabling applications in biosensing, memory, neuromorphic devices, and printed logic circuits. A wide range of organic mixed ionic-electronic conductors (OMIECs), including p- and n-type materials, small molecules, and polymers, have been developed to facilitate ionic and electronic charge transport, ensuring efficient OECT operation. While PEDOT:PSS (poly(3,4-ethylenedioxythiophene):polystyrene sulfonate) has been widely used, its limitations underscore the need for novel OMIECs with diverse properties. Expanding the library of OMIECs is crucial for advancing organic bioelectronics. By modifying the polymer backbone or engineering side chains, OMIECs can achieve tunable electronic, optical, and mechanical properties. In this work, we synthesise a series of semiconducting polymers based on the thienoisoindigo backbone. Through random copolymerization, we systematically explore different donor-acceptor moieties to elucidate their mixed ionic and electronic conduction properties for bioelectronic applications. This study also investigates the structure-property relationship of the thienoisoindigo-loaded polymers in their optical, electrochemical and OECT performance with the help of both experimental and computational approaches.

References

Z. Lu, K. Xu, K. Xiao, Q. Xu, L. Wang, P. Li, J. Zhou, D. Zhao, L. Bai, Y. Cheng and W. Huang, Npj Flex. Electron., 2025, 9, 9.

S. T. Keene, T. P. A. van der Pol, D. Zakhidov, C. H. L. Weijtens, R. A. J. Janssen, A. Salleo and Y. van de Burgt, Adv. Mater., 2020, 32, 2000270.

S. Wang, X. Chen, C. Zhao, Y. Kong, B. Lin, Y. Wu, Z. Bi, Z. Xuan, T. Li, Y. Li, W. Zhang, E. Ma, Z. Wang and W. Ma, Nat. Electron., 2023, 6, 281–291.

Homeotropic alignment study on a two liquid-crystal blend

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The development of organic electronics provides electronic components to the industry that are alternatives to the inorganic semiconductors, but with higher mechanical flexibility, less thickness, weight and cost [1]. Liquid crystal (LC) materials in their mesophases show a molecular organization similar to that of a solid crystal though their viscosity also characterizes them close to a liquid. The main advantage of using LCs as semiconductors is the possibility of controlling the molecular ordering of these materials in relation to the substrate, with molecules aligned face-to-face or edge-to-edge, through thermal treatments [2]. These properties give the semiconductor material a high potential for use in devices, such as Organic Field Effect Transistor (OFETs), Organic Light Emitting Diodes (OLEDs) and Organic Solar Cells (OSCs) [1]. The present work aims to investigate the homeotropic alignment (face-on configuration) in the hexagonal columnar mesophase of a discotic LC consisting of the aromatic center benzo[ghi]perilene-diimide surrounded by peripheral aliphatic chains, referred to here as BPD. To achieve homeotropic alignment in films, different strategies were implemented, such as the formation of blends and bilayer samples with another hexagonal columnar LC (called H4) whose alignment parameters are already known [3]. Thermal treatments in the mesophase were applied to the films, either in open films or in confined films using a sacrificial polymeric layer or glass cells. The results showed domains with dendritic growth characteristic of homeotropic alignment at high temperatures in confined thick films.The effectiveness analysis of those methods was through Polarized Optical Microscopy (POM), photophysical measurements and X-Ray Diffraction (XRD).

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References
[1] Ruiz, C. et al. The Journal of Physical Chemistry Letters, vol. 3, (1428-1436), 2012.

[2] Yilmaz Canli, N. et al. Thin Solid Films, vol. 560, (71-76), 2014.

[3] Eccher, J. et al. ACS Applied Materials & Interfaces, vol.5, (11935–11943), 2013.

Influence of π-Conjugated Polymer Nanoparticles on the Photo- and Thermal Stability of Chitosan Films

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Chitosan films combined with conjugated polymers have attracted attention for sustainable optoelectronic applications [1]. Here, pure chitosan and films incorporating 0.75 wt% nanoparticles of poly(3-hexylthiophene-co-9,9-dioctyl-2,7-fluorene) (PTF) and poly(9,9-dioctylfluorene-co-phenylene) (PFF) were investigated under photo- and thermal degradation. Photodegradation was induced by UV irradiation (254 nm, 48 h), and thermal degradation at 80, 120, and 160 °C (3 h). Structural and optical changes were monitored by UV–vis, infrared, and emission spectroscopy. Under UV irradiation, chitosan films showed a new absorption band at ~300 nm after 6 h, attributed to conjugated carbonyl species formed by oxidative chain scission and deacetylation [2]. In both blend films, this band remained detectable but partially masked by conjugated polymer contributions. Emission spectra broadened due to overlap with degradation products. PFF films exhibited gradual red shift and band broadening, indicating increased emissive heterogeneity likely due to interfacial interactions or conformational disorder [3]. Thermal degradation caused limited changes up to 120 °C, but at 160 °C the ~300 nm band appeared, confirming oxidative chromophore formation. The effect was stronger in PTF films, suggesting facilitated interfacial charge transfer, whereas PFF films showed greater thermal emission stability, consistent with higher rigidity [3]. Overall, degradation depends on the polymer electronic nature, with photodegradation occurring progressively and thermodegradation becoming relevant only at higher temperatures.

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References

[1] M. F. F. das Neves, et al., ACS Appl. Electron. Mater., 7, 3477 (2025).

[2] P. O. Bussiere, et al., Carbohyd. Polym., 259, 117715 (2021).

[3] K. W. Chew, et al., Polymers, 14, 1615 (2022).

Insights into core-level excitations in non-fullerene acceptors

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Near-edge X-ray absorption fine structure (NEXAFS) spectroscopy is a powerful tool to probe the electronic structure of organic semiconductors, yet its interpretation remains challenging for chemically complex systems. In this work, we present a combined experimental and theoretical study of the carbon, nitrogen, and oxygen K-edge NEXAFS spectra of representative non-fullerene small molecule acceptors with A-D-A and A-π-D-π-A structure, such as ITIC and IDTBR, respectively. Angle-resolved NEXAFS measurements are complemented by TDDFT M06/6-311G(d,p) simulations, enabling a detailed assignment of spectral features in terms of core-level excitations, final-state symmetry, and spatial delocalization. The calculations reproduce the experimental spectra with good accuracy and reveal that the number of unoccupied states required for a reliable description strongly depends on the absorption edge, increasing systematically from carbon to nitrogen and oxygen. By correlating transitions across different edges, we show that identical final states can be probed from distinct core levels when heteroatoms are embedded within a conjugated backbone, providing complementary information on the unoccupied electronic structure. Angular-dependent measurements further allow the determination of preferential face-on orientation for these systems. The application of an artificial electric field over the calculated transitions allowed the variation in intensity of the experimental peaks to be reproduced with excellent accuracy, facilitating their understanding and attribution. By providing a unified interpretation of experimental NEXAFS spectra across multiple edges, this work offers new insights into the electronic structure of these acceptors and establishes a robust framework for analyzing core-level excitations in complex organic materials.

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References
SU, G.M. et. al., J. Phys. Chem. C 121, 9142–9152 (2017)

Interaction Between Benzothiadiazolyl triazole Molecules and the Non-Fullerene Acceptor Y18

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The study of the optoelectronic properties of organic molecules is essential for understanding the processes involved in organic photovoltaic devices. In this work, benzothiadiazolyl triazole derivatives, named 1B, 2B, and 3B, and their interactions with non-fullerene acceptor Y18, widely used in organic solar cells (OSC), were investigated. The characterization was carried out in toluene solution using UV–Vis absorption spectroscopy, fluorescence spectroscopy, excited-state lifetime measurements, and fluorescence quenching analysis based on Stern–Volmer models. The absorption spectra showed that the addition of Y18 increases the overall absorbance of the system due to the characteristic absorption bands of these compounds. In addition, the absorption bands of the molecules, particularly in the 320–380 nm region, exhibited slight deformation, suggesting intermolecular interaction between the molecules and Y18. In the emission spectra, progressive fluorescence quenching of 1B, 2B, and 3B was observed with increasing Y18 concentration, while the emission maxima remained practically unchanged at 496 nm (1B), 513 nm (2B), and 527 nm (3B). Lifetime measurements revealed a slight decrease for the 1B + Y18 system, whereas the lifetimes of 2B + Y18 and 3B + Y18 remained essentially unchanged. Stern–Volmer analysis indicated that for 2B and 3B the quenching mechanism is mainly static, suggesting the formation of a non-fluorescent complex. In contrast, the 1B + Y18 system exhibits a combined dynamic and static mechanism. The Stern–Volmer constants obtained were 6.2×10^4, 4.2×10^4, and 5.4×10^4 L mol^{-1} for molecules 1B, 2B, and 3B, respectively, showing higher quenching efficiency for molecule 1B due to the dual quenching mechanism. The higher quenching efficiency observed for the 1B + Y18 system indicates a more favorable interaction between this molecule and the non-fullerene acceptor, making molecule 1B a promising candidate for application in Organic Solar Cells

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References
LAKOWICZ, Joseph R. (Ed.). Principles of fluorescence spectroscopy. Boston, MA: springer US, 2006.

Investigation of solvent-driven chain packing in the bulk of P3HT using MD simulations

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Controlling the morphology of polymeric films remains a challenge in advancing high-performance organic electronic devices. The conformation and packing of polymer chains critically determine the electrical functionality of these devices. A comprehensive understanding of these structural factors is essential for developing the next generation of flexible, printable, and efficient materials applicable to OLEDs, solar cells, transistors, sensors, bioelectronics, and biomimetic systems [1]. As a second-generation semiconducting polymer, P3HT stands as one of the most extensively studied materials of its kind, serving as a benchmark for evaluating new compounds in organic photovoltaic and optoelectronic devices. In this work, we investigate the microstructure of P3HT bulk films using molecular dynamics (MD) simulations with an assisted solvent removal protocol employing a modified all-atom OPLS-AA force field, over 100 ns of simulation trajectories [2]. Our simulations were sensitive enough to demonstrate that solvent choice dictates the morphology of bulk P3HT. While o-dichlorobenzene (ODCB) promoted parallel-displaced stacking through backbone alignment, which favors intermolecular interactions, 1,2,4-trichlorobenzene (TCB) instead induced a more crossing chains distribution. Conversely, when P3HT bulk films were simulated in the absence of solvent, the resulting microstructure exhibited low crystallinity and negligible thiophene ring correlation. This finding reinforces the role of solvent choice as a key factor in film morphology. Furthermore, the ability of our simulation approach to capture the solvent dependence of microstructural behavior, which aligns with experimental observations reported in the literature [3], confirms its utility for materials design.

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References

[1] Ding L, Yu Z-D, Wang X-Y, et al. Chem Rev. 2023;123(12):7421–7497.

[2] Savedra RML, de Morais MNBL, Siqueira MF. J Mol Graph Model. 2022;117:108279.

[3] Kohn P, Rong Z, Scherer KH, et al. Macromolecules. 2013;46(10):4002–4013.

Lignin Biomass Valorisation to High Value-Added Chemicals (phenol and benzaldehyde) using g-C3N4 nanomaterials

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Almost all chemicals around us are obtained from fossil fuels. However, technologies employed to accomplish these chemicals are non-renewable resources and require strong experimental conditions, and therefore, greenhouse gas emissions, impacting global warming and climate change.[1] Biomass is a versatile and renewable resource that produces valuable products using organic waste instead of oil refinery products.[2] Lignin is one of the three major constituents of lignocellulosic biomass. Its structure has a high concentration of C-C bonds due to the presence of aromatic alcohols, which is of interest for the generation of high-value-added chemicals such as phenol or aromatic derivatives. To achieve this, the objective of this research is to obtain direct C-C bond cleavage. In this study, the synthesis of different amounts of α-Fe_2O_3 (0.029% to 3%) on g-C_3N_4 was carried out, and its modification with cyclodextrins (0.29:1 to 2:1) were performed to promote substrate adsorption and therefore a change on the conversion and selectivity. The characterization was carried out by XRD, SBET, IR (, DRS, SEM and TEM among others to confirm the formation of the heterostructures. Bandgaps energies no showed a significantly variation from 2.73 ev for g-C_3N_4 to 2.60 eV for 3% α-Fe_2O_3/g-C_3N_4. The best material 0.1% α-Fe_2O_3/g-C_3N_4 have achieved a conversion of 100% of lignin model at 23h of photocatalysis with a selectivity to phenol of 100% and 29% of benzaldehyde (at 20% of conversion).

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References
Z. Huang, et al., Nat Rev Chem, 6, 197–214 (2022)

M. Wang, at al., Acc. Chem. Res. 56, 1057−1069 (2023).

Mechanistic Origin of Photodegradation and Impurity Effects in Donor–Acceptor Luminescent Radicals

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Organic luminescent radicals have emerged as promising open-shell emitters for advanced optoelectronic and sensing applications. Among them, the carbazole-substituted tris(2,4,6-trichlorophenyl)methyl radical (Cz-TTM) exhibits remarkable photostability and emission efficiency compared with the parent TTM radical. Nevertheless, Cz-TTM can be visibly degraded by indoor light irradiation and its photodegradation mechanism is poorly understood. Here, the study systematically investigates the photochemical behavior of Cz-TTM in solutions, together with the influence of impurities on the photophysical properties of the compound. It is found that emissive and non-emissive impurities are introduced depending on the purification methods and the light irradiation conditions. Impurities cause underestimation of photoluminescence quantum yield through competitive absorption. Photodegradation under continuous irradiation undergoes a multi-step reaction via metastable intermediates, which react with dissolved oxygen upon local excitation of the TTM radical moiety. Quantum-chemical calculations indicate a ring-closure followed by dechlorination within the TTM moiety as the key degradation pathway. The superior photostability of Cz-TTM to TTM originates from its stabilized first excited doublet energy level, which increases the activation energy for ring-closure reaction in Cz-TTM. These combined experimental and theoretical insights reveal the fundamental factors governing the photostability of TTM-type luminescent radicals and offer design principles for next-generation organic luminescent materials [1].

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References
[1] T. Hosokai, et al., Adv. Opt. Mater. 14, e03832 (2026)

Modulating Anti-Kasha Fluorescence and Phosphorescence in Azulene Derivatives

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According to Kasha's rule, the emitting level is the lowest in energy of a given multiplicity, i.e., S1. Azulene was the first molecule that showed anti-Kasha fluorescence, i.e. emits from a higher excited state level, i.e., S2. The high interest in this phenomenon lies in the possibility of modulating the energy of the high energy emitting states, which can open new possibilities in constructing new molecular materials with different potential applications. Several studies have tried to explain the structure-property relationship to modulate anti-Kasha properties, however, they remain inconclusive. For this purpose, different azulene-based molecules have been studied by different spectroscopic techniques, such as low-temperature absorption/emission and transient absorption spectroscopy. These techniques represent the perfect tools to elucidate the structure-property relationship to improve the design of organic materials. Among all these molecular structures, azuacenes demonstrate the modulation of anti-Kasha fluorescence by conjugation. [1] In addition, attaching carbazole to azulene induces triplet population followed by anti-Kasha phosphorescence. Finally, azuperylene [2] and its characteristic anti-Kasha phosphorescence is discussed. This work, therefore, displays some recipes to modulate anti-Kasha phenomena by varying the molecular structure of azulene derivatives. [1-3]

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References

[1] M. Díaz-Fernández, F. Huang, J.M. Marín-Beloqui, L. Sun, Y. Chen, S. Liu, Y. Wang, H. Zheng, S. Li, C. Zhang, J. You, J. Casado. J. Am. Chem. Soc., 147,1574-1583 (2025).

[2] S. Liu, M. Díaz-Fernández, M. Zhang, F. Huang, Y. Chen, Y. Yang, J.M. Marín-Beloqui, J. Lang, J. You, J. Casado, C. Zhang. Angew. Chem. Int. Ed., 64, e202505897 (2025).

[3] A. Diaz-Andres, J. Marín-Beloqui, J. Wang, J. Liu, J. Casado, D. Casanova. Chem. Sci., 14, 6420-6429 (2023).

Modulation of Photoinduced Electron Transfer by Sulfur-to-Selenium Substitution in Benzazole Systems: A Fluorescence Quenching Study

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Structural modification through heteroatom substitution represents an effective strategy to tune the electronic properties of conjugated organic systems. In this work, we investigate how sulfur–selenium substitution influences photoinduced electron transfer (PET) in two structurally analogous benzazole fluorophores: BST (sulfur-containing) and BSe (selenium-containing). Steady-state fluorescence measurements revealed significant emission quenching in the presence of electron acceptors, with behavior well described by the Stern–Volmer model. For BST, Stern–Volmer constants (Ksv) of 4.3×10^3 L·mol^{-1} (C60), 8.0×10^3 L·mol^{-1} (PyC60), and 5.1×10^4 L·mol^{-1} (Y18) were obtained. In comparison, BSe exhibited Ksv values of 3.4×10^3 L·mol^{-1} (C60), 5.3×10^3 L·mol^{-1} (PyC60), and 5.8×10^4 L·mol^{-1} (Y18). Although both systems display high quenching efficiency, the heteroatom identity distinctly modulates donor–acceptor electronic coupling in the case of fullerene-based acceptors, while maintaining comparable efficiency toward the non-fullerene acceptor. Bimolecular quenching rate constants (Kq) associated with Y18 reached values on the order of 10^{12} L·mol^{-1}·s^{-1} for both fluorophores, indicating highly efficient processes approaching the diffusion-controlled limit. The quantitative differences observed between BST and BSe suggest that the increased polarizability and modified electronic distribution introduced by selenium influence excited-state donor–acceptor interactions. These results demonstrate that sulfur–selenium substitution acts as a relevant structural parameter in modulating electron transfer efficiency in benzazole systems, contributing to a deeper understanding of structure–photophysics relationships in functional organic materials.

Acknowledgements
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References
Lakowicz, J. R.; Principles of Fluorescence Spectroscopy, 3rd ed.; Springer: Boston, 2006.

Molecular modeling of arylazopyrazole surfactants: photophysical and self-assembly properties

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Azo-based molecules can act as photoresponsive materials when they absorb specific wavelengths and undergo reversible conversion between their trans-cis (E → Z) isomerization. This molecular switching has enabled their widespread application across diverse fields, including drug delivery, photopharmacology, energy storage, and the development of adaptive biotechnological materials [1,2]. Traditionally, azobenzenes have set the standard for light-induced isomerization. However, arylazopyrazoles are redefining these limits by enabling near-total E-to-Z conversion, overcoming the incomplete switching often observed with conventional derivatives. The self-assembly of isomers of an arylazopyrazole-based photosurfactant was investigated using Quantum Mechanics (QM) and Molecular Dynamics (MD) simulations, in water [3]. The electronic structure calculations were performed using the DFT approach, at the PBE0/cc-pVTZ level. To investigate molecular self-assemblies, we used a modified all-atom OPLS-AA force field throughout 260 ns of simulation trajectories. The frontier orbitals of the isomers exhibited distinct electronic distributions, influencing both the bandgap and the nature of electronic transitions. Initial models started from random molecular distributions in cubic boxes of the same dimensions (10 nm edge length). The Z isomer condensed into a quasi-spherical aggregate, whereas the E isomer yielded an ellipsoidal configuration and showed a significantly slower rate of stabilization. These micelle formations agree with reported experimental results [2]. Furthermore, the radial distribution functions (RDF) plots show that both final structures adopted micellar morphologies, characterized by a dense hydrophobic core and a well-defined hydration shell at the interface. These findings demonstrate that our molecular modeling approaches provided important insights into the self-assembly of these photoresponsive materials at the molecular level.

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References
[1] M. Gao, et al., Nat. Sci. 3, e220020 (2023).

[2] G. Tyagi, et al., JACS Au 2, 2670 (2022).

[3] R. M. L. Savedra and M. F. Siqueira, J. Mol. Liq. 398, 124255 (2024).

Monte Carlo Modeling of Flexible Amphiphile Self-Assembly: Energetics, Chain Stiffness, and Micelle Formation

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Understanding micelle-mediated morphology control in surfactant-assisted sol–gel systems requires addressing the complexity of mixed surfactant formulations, where amphiphiles with different chain lengths, interaction strengths, and molecular flexibility coexist [1,2]. A lattice-based Monte Carlo framework is proposed here and has been developed to investigate competitive self-assembly in mixed amphiphile populations. Amphiphiles are represented as flexible head–tail chains with variable tail lengths and interaction parameters on a two-dimensional lattice with excluded-volume constraints [2]. Multiple species are simulated simultaneously to explore the effects of polydispersity and competitive aggregation. Preliminary simulations indicate that the cross-interaction strength between amphiphile species governs the aggregation regime. When the cross-interaction energy approaches the average self-interaction energy, mixed micelles dominate, representing ~70–85% of aggregates with stable compositional ratios. For weaker cross-interactions, segregation occurs and cluster purity exceeds ~90%, producing micelles composed primarily of a single species. Intermediate regimes exhibit selective incorporation, where large mixed micelles coexist with smaller single-species aggregates, leading to bimodal cluster-size distributions. Time-resolved analysis reveals metastable coexistence of states and slow to reach equilibrium at around 10^5–10^6 Monte Carlo steps. These results provide quantitative insight into how different surfactants interact differently and how they influence micelle composition and aggregation pathways, offering guidance for controlling nanoscale morphology in solution-processed thin films, which seems a rather low-cost key for electronic devices.

Acknowledgements
FAPES 2022/13479-1

References

G. Puača, V. Tepavčević and M. Poša, J. Chem. Thermodyn. 173, 106835 (2022)

J. N. Israelachvili, D. J. Mitchell and B. W. Ninham, J. Chem. Soc., Faraday Trans. 2 72, 1525 (1976)

D. W. Cheong and A. Z. Panagiotopoulos, J. Phys. Chem. B 110, 17915 (2006)

Multifunctional Discotic Liquid Crystals Based on Acylhydrazones

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Liquid crystals (LCs) are a distinct state of matter characterized by ordered structures and unique physical properties, making them important for both fundamental research and technological applications [1]. The incorporation of acylhydrazone units significantly broadens the functionality of liquid crystalline systems by promoting organogel formation, enabling metal coordination, and providing reversible photoisomerization, thereby allowing remote modulation of material properties. Additionally, supramolecular aggregation in π-conjugated systems can influence their electronic behavior, making these materials promising platforms for multifunctional supramolecular systems [2]. Therefore, discotic molecules containing three acylhydrazone groups with C3 symmetry were synthesized to expand the group's current studies on these materials [3] and to investigate how the direction of the acylhydrazone group and variations in shape and number of flexible chains affect their mesomorphic, photophysical, and photoisomerization properties. The synthesis of the materials was confirmed by ^{1}H and ^{13}C NMR and elemental analysis, whereas their thermal and LC behavior investigated by TGA, DSC, POM, and XRD techniques. POM and DSC analyses showed that compounds with nine peripheral alkoxy chains behave as ordinary solids, while materials with six alkoxy chains exhibited highly viscous hexagonal columnar (Colh) LC phase, which was further confirmed by XRD measurements. The photoisomerization behavior of the materials was studied using ^{1}H NMR and UV–Vis absorption spectroscopy. Under UV irradiation, all compounds showed a decrease in the absorption band of the E isomer and the appearance of bands associated with the Z isomer, along with hypsochromic shifts, confirming the E–Z photoisomerization process. Both compounds showed aggregation induced emission in solvent mixtures of THF and water and complexation to Pd2+ cations and were able to form organogels in some solvents.

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References

H.K. Bisoyi, Q. Li, Liquid Crystals: Versatile Self-Organized Smart Soft Materials, Chem. Rev. 122(5), 4887-4926 (2022).

Babu, S. S., Praveen, V. K. & Ajayaghosh, A. Functional π-Gelators and Their Applications. Chem. Rev. 114, 1973–2129 (2014).

W.A. de Oliveira, M. Alaasar, Y. Cao, E. Westphal, 1,4-Bis(Acylhydrazone)-Based Polycatenar

Liquid Crystals: Self-Assembly, Molecular Switching, and Gelation Properties, ACS Omega 10(21), 21637-21647 (2025).

Organic and flexible colorimetric sensor for the detection of copper ions in water and Cachaça

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Copper is essential to the human body; however, when consumed in excess, it becomes harmful to health. In this work, we developed printed colorimetric sensors using the flavonoid quercetin, incorporated into cellulose acetate, to detect and quantify permissible concentrations of Cu^{2+} ions in water, ≤ 2 mg/L per day, and Cachaça (Brazilian sugarcane spirit), ≤ 5 mg/L). Quercetin contains an extended π-conjugated aromatic system in which electrons are delocalized across multiple rings. This delocalization creates low-energy π→π* transitions that are highly sensitive to coordination with metal ions. Upon complexation with Cu^{2+}, the electron density of the conjugated system is perturbed, altering the energy gap between π and π* orbitals and producing measurable color changes in the films. This mechanism makes flavonoids attractive π-conjugated materials for visual metal sensing. Sensors with different geometric designs were fabricated by combining copper-sensitive and non-sensitive films, enabling the formation of multitoned images derived from a single base color. The sensors exhibited color variations from yellow-green to dark yellow for copper levels between 0 and 90 mg/L, and from yellow-green to light yellow or cream for the ranges of 0–2 mg/L (water) and 0–5 mg/L (cachaça). The devices showed high optical stability (~1 year), linear response, simple color reading, thermal stability, and response times of 20 min for water, and 8 min for cachaça. These results highlight the potential of π-conjugated molecules in printed and flexible colorimetric devices for inspecting and controlling the quality of water and beverages contaminated with copper.

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References

FIGUEIREDO, Matheus Torres Duarte et al. Immobilization of anthocyanin in polymeric film to obtain a colorimetric sensor for detection of copper in cachaça. Food Analytical Methods, v. 15, n. 12, p. 3535-3553, 2022.

HEIM, Kelly E.; TAGLIAFERRO, Anthony R.; BOBILYA, Dennis J. Antioxidantes flavonoides: química, metabolismo e relações estrutura-atividade. The Journal of nutritional biochemistry , v. 13, n. 10, p. 572-584, 2002.

AZEEZ, Luqmon et al. Syntheses, characterizations and antioxidant activities of copper complexes of quercetin as influenced by redox states. International Journal of Biological and

Chemical Sciences, v. 9, n. 5, p. 2712-2718, 2015.

Organic Hyperbolic Materials for Optoelectronic Applications

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Hyperbolic metamaterials are artificially structured dielectric/metal materials whose principal components of the dielectric permittivity tensor have opposite signs, producing a hyperbolic dispersion relation that enables propagation of high-wavevector modes, strongly modified local density of states and unusual light–matter interactions. Uniaxial anisotropic organic materials (OHMs) showing hyperbolic dispersion in neat films could represent a promising alternative to conventional inorganic metamaterial platforms and open new opportunities in the field of organic optoelectronics In a previous study, polycrystalline thin films made of the quinoidal oligothiophene, QQT (CN)4, was found to naturally exhibit hyperbolic dispersion in the near-infrared (NIR) region. [1] However, only a very limited number of molecular structures have been reported to exhibit hyperbolic dispersion in the visible spectral range. Here, we present a new π-conjugated molecule based on a squaraine backbone that shows hyperbolic dispersion in the visible region. Spin-coated films of this material demonstrate characteristic H-aggregation feature in their absorption spectra, leading to hyperbolic dispersion around 515nm. Reflectivity dip for p-polarized light observed in attenuated total reflection (ATR) measurement further supports the presence of surface exciton polaritons (SEPs) in the films.

References

[1] Y. U. Lee, A. D'Aleo, J-C Ribierre et al., ACS Photonics, 6 (7), 1681-1689 (2019)

Organic π-Diradicals in Action

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Diradical molecules have been prepared in the last 10 years in chemically stable modes opening the window for their applications in organic electronics [1]. Examples of their devices are organic field-effect transistors (i.e., OFETs), in non-linear optics, in photovoltaics, in photodynamic applications, in spintronics, etc. In most of these investigations, the connection between the function and the intrinsic diradical electronic structure is not well stablished, or not discussed in sufficient detail, what often limits very much further optimization of the corresponding device and the progress in the refinement of their chemical and electronic structures. In the last times, we have been interested in the understanding of the spectroscopic and electronic properties of diradicals from the very basic point of view and realized of significant connections between the degree of two electrons unpairing (i.e., diradical character) and the energy disposition and nature of the ground electronic and of the lowest energy lying excited states [2]. In this communication, examples of diradicals implemented in organic electronic devices will be presented and their intimate electronic properties discussed in the context of their functions [3]. The studied diradicals are based on Blatter radicals, in difluorenoheteroles, in bisindene diradicals and in azacene diradicals

Acknowledgements
The authors acknowledge the Spanish government for financial support (project PID2024-157601NB-I00)

References
[1] J. Liu, X. Feng, Angew. Chem. Int. Ed. 59, 23386-23401 (2020)

[2] M. Haley, M. Kerstez, J. Casado, Angew. Chem. Int Ed. 134, e202209138 (2022)

[3] J. Casado. U. Bunz, et al. Angew. Chem. Int. Ed. 62, e202305712 (2023)

Perylene Diimide Encapsulation with the Mechanical Bond

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Perylene diimide (PDI) is an organic chromophore that has received significant attention for a wide range of organic (opto)electronic applications.[1] It is a strong electron acceptor, making it attractive for use as an n-type semiconductor; also its strong absorption and emission in the visible region make it a good candidate for organic solar cells and LEDs.

Synthetic modification of the imide and perylene core positions of the PDI have been widely reported and the effects on physical and electronic properties are well understood.[2] Aside from such covalent modifications, mechanical bonding is underexplored as a strategy for controlling PDI electronics and intermolecular interactions. A mechanical bond is generated through the interlocking of [n] molecular components that cannot be separated without breaking a covalent bond, with archetypal structures being [n]rotaxanes and [n]catenanes.

Complementing covalent strategies,[3] we investigate the mechanical interlocking of PDI as a method of chromophore encapsulation, allowing control over its aggregation and susceptibility to photodegradation, both of which are advantageous in the context of device applications. Mechanical bonding also provides the potential to tune the non-covalent interactions between the interlocked components, interactions that may otherwise be too weak to be observed in analogous intermolecular systems. Therefore, this presentation will discuss the impact of interlocking a PDI with either one (i.e., a [2]rotaxane) or two macrocyclic rings ([3]rotaxane), including with macrocycles that are capable of π-stacking with the chromophore's perylene core.

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References

C. Huang, S. Barlow and S. R. Marder, J. Org. Chem., 2011, 76, 2386-2407

A. Nowak-Król and F. Würthner, Organic Chemistry Frontiers, 2019, 6, 1272-1318

E. M. Holdsworth, H.-H. Cho, A. D. Bond, S. Montanaro, S.-J. Woo, T. Huang, J. Shaikh, F. Hassan, S. Gorgon, V. Riesgo-Gonzalez, A. J. Gillett, D. G. Congrave, R. H. Friend and H. A. Bronstein, Journal of the American Chemical Society, 2026, 148, 8163-8173

Photoinduced Enhancement of Fluorescence Quantum Yield in an Isoxazoline–Carbazole Derivative

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Carbazole-based organic compounds have attracted considerable attention for optoelectronic applications due to their chemical versatility and favorable photophysical properties. Carbazole derivatives exhibit high thermal stability and molar absorption coefficients on the order of 10^4 L·mol^−1·cm^−1 [1], displaying absorption and fluorescence in the UV–Vis region and acting as efficient hole-transporting materials in optoelectronic devices such as Organic Light-Emitting Diodes (OLEDs) [2]. In this study, the photophysical properties of carbazole–isoxazoline derivatives were investigated in acetonitrile solution (10^−5 mol·L^−1) bearing phenyl (1a), chlorophenyl (1b), bromophenyl (1c), and aldehyde (1g) substituents. Spectroscopic measurements revealed absorption bands at 233, 289, and 330 nm and fluorescence emission centered at 342 nm, attributed to the carbazole moiety. A molar absorption coefficient on the order of 10^4 L·mol^−1·cm^−1 at λ = 290 nm, a Stokes shift of 970 cm^−1, and an excited-state lifetime of 7 ns were observed. All compounds exhibited photoinduced increase in fluorescence quantum yield upon UV irradiation, with enhancement factors of 2.1, 5.4, 3.4, and 4.6 for 1a, 1b, 1c, and 1g, respectively. However, oxidation of the isoxazoline moiety in chlorophenyl (2b) and bromophenyl (2c) derivatives produced isoxazole structures with increased rigidity. Despite similar absorption and fluorescence profiles, the photoinduced fluorescence enhancement observed for isoxazoline derivatives was absent after oxidation. These results indicate that the conformational mobility of the isoxazoline moiety is crucial for this effect, as supported by computational simulations. The variation in fluorescence quantum yield indicates the potential of these compounds for new applications in optoelectronic devices.

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References

Tao, Y. et al. New J. Chem. 2025, 49, 935–942.

Graebe, C.; Glaser, C. Justus Liebigs Ann. Chem. 1872, 163, 343–362.

Valeur, B.; Berberan-Santos, M. N. Molecular Fluorescence; Wiley-VCH, 2012, 75–107.

Quantum Yield of Perylene-Derived Emitters Improved by Crystalline Liquid Host Alignment

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Organic light emitting diodes (OLEDs) can currently achieve 100% internal quantum efficiency. However, the external quantum efficiency of the device is limited by the poor extraction of photons. Molecular alignment with the emitter dipole moment parallel to the surface has been demonstrated to improve light outcoupling[1,2]. We investigated the role of a triazine columnar liquid crystal as self-assembling anisotropic host compared to non-liquid crystalline hosts DPEPO and PMMA. Films were prepared onto quartz from chloroform solutions in ratio of 1% in moles, in PMMA 1% by mass. Measurements of absorption, emission, quantum yield and photoluminescence lifetime were performed for photophysical characterization. XRD analyses were performed to characterize the molecular organization. TD-DFT was used to identify the transitions to the excited state. Two perylene derivatives were studied as guests, one of them itself a columnar liquid crystal at room temperature. Their spectral overlap with the liquid-crystalline host favored Förster Resonance Energy Transfer (FRET). The ability of the host to induce columnar aggregates was observed, resulting in higher photoluminescence quantum yields (PLQY) when compared to non-liquid crystalline hosts. The columnar host improved FRET with photoluminescence quantum yields (PLQY) of the guest emitters up to 84% due to host excitation, which is higher than the PLQY with direct guest excitation. The result of favoring the FRET of the host to the emitters at the edges of the columnar aggregates reduces the losses due to non-radiative decay, which is more frequent inside the aggregates. In conclusion, an anisotropic columnar liquid-crystalline host improved light outcoupling due to horizontal guest alignment and increased PLQY due to FRET for guests with lower non-radiative loss.

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References
Kim, K.-H. and J.-J. Kim. Advanced Materials, 2018. 30(42): p. 1705600.

Eccher, J., et al. ACS Applied Materials & Interfaces, 2013. 5(22): p. 11935-11943.

Silicon Phthalocyanines: From Air Stable N-Type To Record Breaking P-Type Performance In OTFTs

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Silicon phthalocyanines (SiPcs) are a distinctive and underexplored class of phthalocyanines in which axial ligation at the silicon center provides unusual control over both molecular and solid-state properties. In contrast to metal-centered phthalocyanines, axial substitution in SiPcs enables systematic tuning of solubility, intermolecular interactions, and thin-film organization without substantially altering the macrocycle's electronic structure or optical absorption. This decoupling of molecular packing from frontier orbital energies makes SiPcs a powerful platform for establishing clear structure–property relationships. Organic thin-film transistors (OTFTs) based on SiPcs demonstrate that axial functionalization directly governs key device parameters. For example, increasing the electron-withdrawing character of the axial substituents systematically reduces threshold voltages over nearly an order of magnitude while maintaining electron mobilities exceeding 0.5 $cm^2\ V^{-1}\ s^{-1}$, among the highest reported for phthalocyanines. To systematically link molecular structure, processing conditions, and device behavior, we employ high-throughput fabrication and characterization approaches that enable rapid exploration of the multidimensional parameter space associated with organic semiconductors. Using automated, on-chip fabrication of OTFTs, we map the influence of deposition parameters across multiple SiPc derivatives, establishing clear correlations between processing conditions, thin-film structure and charge transport. Recently, we have shown that fabrication parameters influence both the initial film structure and its thermal response, enabling the design of more thermally resilient organic electronic devices. These results position silicon phthalocyanines as a chemically tractable platform where molecular design controls structure, processing, and electronic function, linking synthesis to device-relevant properties.

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References

Small Methods, 2025, e00782

Advanced Functional Materials, 2024, 2408779

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Solvent and Solid-State Effects on the Photophysical Properties of Benzothiadiazole and Benzoselenadiazole Derivatives

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This work presents a systematic investigation of the photophysical properties of 4,7-bis(phenylethynyl)[2,1,3]benzothiadiazole (BST) and 4,7-bis(phenylethynyl)[2,1,3]benzoselenadiazole (BSe) under different environmental conditions. The influence of solvent polarity, specific solute–solvent interactions, and solid-state organization on their optical behavior was evaluated through absorption and fluorescence spectroscopy. In solvents with varying polarity, a linear correlation between Stokes shift and solvent polarity parameters was observed for most aprotic solvents, encompassing both polar and nonpolar media. This behavior indicates stabilization of the excited state by nonspecific dipolar interactions. In contrast, protic solvents and oxolane exhibited deviations from linearity, suggesting the contribution of specific intermolecular interactions affecting the excited-state relaxation dynamics. In the solid state, optical bandgap (Egap) values of 2.76 eV for BST and 2.31 eV for BSe were determined, reflecting the influence of chalcogen substitution on electronic structure and intermolecular packing effects. Radiative (kr) and non-radiative (knr) decay rate constants were also analyzed, providing insight into the balance between emissive and non-emissive deactivation pathways. The selenium-containing derivative exhibited distinct decay dynamics consistent with enhanced electronic delocalization and modified excited-state characteristics. The combined results reveal a strong structure–environment interplay governing the emission behavior of these benzazole systems, highlighting the role of heteroatom substitution and medium effects in tuning their optoelectronic properties.

Acknowledgements
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References
Lakowicz, J. R.; Principles of Fluorescence Spectroscopy, 3rd ed.; Springer: Boston, 2006.

Strategic Design of Optically Active Molecules: The Impact of Central and Peripheral Group Substitutions

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Optically active liquid-crystalline materials are fundamental to the innovation and performance of modern emission devices. A detailed understanding of the radiative decay dynamics is essential for comprehending photophysical phenomena observed during operation, while also serving as an important guide for the strategic design of new synthetic pathways. In this work we used Density Functional Theory (DFT) [1] calculations to characterize molecular orbitals and map electronic transitions, by considering changes in central and peripheral groups. The resulting theoretical predictions were rigorously compared and validated against experimental data. Findings are driven by the nature of the low-lying excited states and the localization of the frontier orbitals and how the molecule's shape and internal angles impact its properties. The substitution of a central amid for an ester group enforces an increase in the main centralized dihedral angle which localizes electronic transitions and induces a pseudo-symmetry in the frontier orbitals. These changes fundamentally influence the photophysical behavior and are correlated with the photoluminescence quantum yield in solution. By mapping these specific electronic and optical properties, this research offers a theoretical framework for the design of high-performance molecules for optical devices.

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References
[1] K. Capelle. Brazilian Journal of Physics, 2006, 36(4 A), pp. 1318-1341

Substituted Trichlorotriphenylmethyl-based Radicals: Design, Synthesis and Photophysical Properties

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Organic light-emitting diodes (OLEDs) have gained widespread attention in both scientific research and commercial applications due to their low cost, flexibility, environmental friendliness, and ease of processing. For traditional closed-shell molecular systems, according to quantum spin statistics, electrons and holes recombine in the luminescent layer at a ratio of 1:3 to form singlet and triplet excitons. OLEDs can only utilize up to 25% of singlet excitons for luminescence, while the triplet excitons, which account for up to 75%, are usually non-luminescent due to spin prohibition, resulting in a large number of wasted excitons. There are well-known strategies for utilizing triplet excitons such as triplet−triplet annihilation (TTA), hybridized local and charge-transfer (HLCT) and thermally activated delayed fluorescence (TADF), but these systems all have downsides like device life and stable working efficiency. Unlike focusing on closed-shell systems, a promising direction is to use open-shell radical systems as emission layers. Radical molecules have an unpaired electron, and both their ground state and excited state are doublet states, which can avoid the problem of triplet exciton transition forbiddance and theoretically achieve 100% internal quantum efficiency without intersystem crossing. Triphenylmethyl-based radicals are one of the few types of radicals with relatively high stability. Introducing electron donors as substituents on trichlorotriphenylmethyl (TTM) radicals to design donor−acceptor (D-A) type molecules is a widely adopted strategy to improve radical stability and quantum efficiency [1].

Acknowledgements
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References
Li, P. et al. The Journal of Physical Chemistry A 128 4279−4287 (2024)

Synthesis and application of D-A-D fluorescent organic molecules in luminescent solar concentrators (LSCs), visible light communication (VLC) and photocatalysis.

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Organic fluorophores with donor–acceptor–donor (D-A-D) structures exhibit peculiar optical properties. They are typically characterized by strong absorption in the visible range, a large Stokes shift, and a high fluorescence quantum yield. In addition, they are generally easy to synthesize using scalable synthetic methodologies. We recently synthesized and investigated a series of organic fluorophores with D-A-D structures, employing quinoxaline (DQ)[1], benzo[1,2-b:4,5-b′]dithiophene 1,1,5,5-tetraoxide (BDT)[2], dithieno[3,2-b:2′,3′-d]thiophene-4,4-dioxide (DTT)[3] and dithienoditieno [3,2-b;2’,3’- d]phosphole (DTP) as central acceptor cores. The optical characteristics of these materials enabled their application in optical devices such as luminescent solar concentrators (LSCs). LSCs are large-area optical devices capable of harvesting, downshifting, and concentrating solar radiation through the use of emitting materials embedded in a polymer matrix. These materials can be combined with silicon-based photovoltaics (PV) to fabricate devices capable of efficiently capturing diffuse light. Their tunable aesthetic features (color and shape) further support their use in building-integrated photovoltaics (BIPVs). Additionally, the same devices can serve as antennas in visible light communication (VLC), one of the most promising candidates for next-generation 6G communication technologies. The best-performing LSCs fabricated with the fluorophores developed by us exhibited photonic and photovoltaic efficiencies comparable to state-of-the-art devices. Furthermore, we demonstrated efficient VLC operation using these fluorophores.

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References

Papucci, C.; et.al J. Mater. Chem. C. 2021, 9, 15608.

Bartolini, M. et.al ACS Appl. Energy Mater, 2023, 6, 4862.

Bartolini, M. et.al ACS Appl. Energy Mater. 2025, 8, 5317

Synthesis and evaluation of novel D-A-D and A-D-A fluorene-based photosensitizers for DSSC

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DSSCs (Dye-Sensitized Solar Cells) are devices capable of converting solar energy into electrical energy through semiconductor nanoparticles sensitized by dyes. In order to propose more sustainable and less expensive options, there is a growing interest in the development of efficient metal-free photosensitizers, produced through simpler synthetic routes [1]. The development of purely organic dyes aims at constructing a structure in which an electron-donor group is linked to a conjugated bridge, which in turn is connected to an electron-acceptor group capable of anchoring to the semiconductor (usually TiO_2) [2]. This work was based on the synthesis and characterization of new dyes using fluorene as the conjugated bridge, aiming to obtain suitable photosensitizers for DSSCs. Four fluorene derivatives were synthesized using different donor and acceptor groups in two molecular architectures: D–A–D for 2TPA-CA and A–D–A for TPA-2CA, TPA-2CYA, and DPA-Th-2CYA. The synthesis of these compounds has 2,7-dibromofluorene as its starting material, which was submitted to a Knoevenagel condensations using different aldehydes, followed by a Suzuki cross-coupling reaction. Photophysical studies of absorption and emission in solution were carried out, in addition to solid-state reflectance measurements via DRUV-Vis. The compounds exhibited high molar absorptivity values in solution ($\varepsilon \sim 10^4$ L mol^{-1} cm^{-1}). Furthermore, all compounds were applied in the sensitization of DSSCs in order to evaluate their photo-conversion efficiencies (η) and compare them with the ruthenium complex N719, one of the best commercial dyes. The synthesized compounds showed η values ranging from 0.41% to 2.23. The obtained results highlight the potential of fluorene as conjugated scaffold for the development of new photosensitizers, especially in the A–D–A architecture, which remains underexplored in the literature.

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References

Yen, Y. S.; Chou, H. H.; Chen, Y. C.; Hsu, C. Y.; Lin, J. T.; J. Mater. Chem. 2012, 22, 8734.

Kakiage, K.; Aoyama, Y.; Yano, T.; Oya, K.; Fujisawa, J. I.; Hanaya, M.; Chem. Commun. 2015, 51, 15894.

Thienothiophene Based Conjugated Materials for Organic Electronics

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Thienothiophene (TT) and dithienothiophene (DTT) are fused thiophenes, composed of two and three annulated thiophene rings, respectively, for TTs and DTTs. TTs and DTTs have extended p-conjugation, planar structure, intermolecular S---S interaction, and electron rich, flat, rigid, and good electron delocalized skeleton. These properties make them very suitable and desirable main building blocks for organic electronics.TTs and DTTs have been attracted a great interest in material chemistry as both polymeric and small molecules for organic electronics such as organic light emitting diodes (OLED), organic field effect transistors (OFET), organic solar cells (OSC), capacitors and sensors. In this work, some recent TT and DTT units having various functional groups, developed by our research group, and their use in organic electronic and optoelectronic applications are summarized.

References

R. Isci, K. B. Donmez, N. Karatepe, T. Ozturk, ACS Appl. Energy Mater. 7 (2024) 1488-1494

M. E. Cinar, and T. Ozturk, Chem. Rev. 115 (2015) 3036-3140

R. Isci, K. B. Donmez, Z. Cobandede, B. Chakrabarti, N. Karatepe, T. Ozturk, J. Mater. Chem. A 13 (2025) 39887-39902

Tris(aryloxadiazolyl)triazines and Tris(aryloxadiazolyl)benzenesAnalogous stars with different mesomorphic behavior

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C3-symmetrical mesogenes with aryl-1,3,4-oxadiazole arms form broad liquid crystalline mesophases and show the characteristic textures of a columnar arrangement as observed by POM. 1,3,4-Oxadiazoles are accessible from tetrazoles and carbonyl chlorides via Huisgen-reaction.[1] A series of stars with systematically varied substitution pattern and chain length has been synthesized.[2] Molecular structure, thermotropic behavior and optical properties were studied. All tris(aryloxadiazolyl)triazines and -benzenes are fluorescent molecules with excellent columnar arrangement in the LC phase and broad mesophases. These materials in their LC phase show characteristic fan textures and pseudo focal conic fans in POM. The width of the mesophases of tris(phenyloxadiazolyl)triazines range from 85°C to 180°C for the 3,4-derivates and even up to -10°C to 210°C for the 3,4,5-trioctyloxy homologue but the phase widths of benzene-analogues are about 40°C smaller. XRD on oriented fibres in combination with experimentally determined density clarified that the packing of the 3,4,5-derivatives is more dense than of the 3,4-derivatives. For 3,4,5-substituted triazines with 18 alkyl chains per aromatic core, the space between the formed columns is completely filled. Due to stronger π-π-interactions the melting points of 3,4-derivatives are higher than of the 3,4,5-analogues. In the mesophase all compounds assemble in the columnar hexagonal structure with ca. 3.5 Å π-π-distances, resulting in one wide-angle reflex. Transition of triazine compounds from the crystalline to the liquid crystal phase reduces the intercolumnar distances. Shrinking of the lattice constants is compensated by an increase of the π-π-distances. Benzene analogues undergo massive structural changes during melting due to higher intra- and intercolumnar variation, which results in higher melting points than triazine compounds. Benzene stars are colourless, triazines yellow to red and fluoresce in the visible range.

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References
R. Huisgen, H.J. Sturm, M. Seidel, Chem. Ber., 1961, 94, 1555.

N. Tober, T. Rieth, M. Lehmann, H. Detert, Chemistry (2019) 25, 15295

Tris(N-phenyltriazole) Liquid Crystalline Matrices for Anisotropic Emission

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Although Organic Light Emitting Devices (OLEDs) are widely used today, they still suffer from significantly low efficiency, leaving substantial room for further development. For this purpose, alignable liquid crystals made of disk-shaped molecules hold great potential for OLEDs, as aligning the emitter dipoles relative to the device surfaces can significantly reduce losses caused by inefficient light outcoupling.[1] However, an effective matrix (host) for thermally activated delayed fluorescence (TADF) emitters must possess a triplet excited state energy higher than that of the emitting guest molecules, thereby avoiding energy transfer losses. Ideally, the T1 state energy should be around or above 3 eV to allow emission at all visible wavelengths. Thus, the design of new materials should consider the combination of molecular self-alignment and precisely tuned photophysical properties. Tris(N-phenyltriazoles) (TPT) is a rigid core that exhibits planarity and electron-withdrawing character, and it has still been little used in organic electronics. [2] By combining the planar structure of TPT with viscosity-inducing ester units, it is possible to obtain liquid crystals with different organizations depending on the position of the ester chain. While the ester group at meta position (TPT3Cn) favors nematic columnar behavior, the para position (TPT4Cn) favors columnar hexagonal ordering. The chain length has a slight influence on the stability of the mesophase, favoring mesomorphism as the chain length increases. Through solid-state emission experiments at 60 K, it was observed that the photophysical behavior is also slightly influenced by the position of the ester group, since there is no significant difference between the T1 energy of the TPT3C3 and the TPT4C3. These results highlight the promise of the TPT core as a platform for developing liquid-crystalline matrices with tailored photophysical properties for the alignment of emissive layers in optoelectronic devices.

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References
D. Yokoyama, J. Mater. Chem., 21, 19187-19202, (2011)

C. Ratto, Mol. Cryst. Liq. Cryst. 657, 147–155 (2017)

(Photo)catalytic doping of organic semiconductors

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Keywords: chemical doping, catalytic doping, photocatalysis, redox chemistry.

Chemical doping in organic semiconductors is governed by a complex interplay of redox energetics, charge-transfer kinetics, and ion stabilization. Achieving high charge densities and electrical conductivities requires not only efficient electron transfer but also control over reaction pathways and transient intermediates, as well as over how the resulting charges are stabilized by counterions. Most established doping strategies rely on highly reactive oxidants or reductants that directly transfer charge to the semiconductor. While effective, these dopants are often difficult to control and can compromise selectivity, stability, or processing compatibility. In this presentation, I will highlight some of our recent work exploring catalytic approaches to doping organic semiconductors. By using metal catalysts, light-driven redox cycles, and reactive intermediates generated in situ, we decouple dopant strength from intrinsic chemical reactivity. This enables doping under milder conditions with weak or readily available reagents, while offering better control over reaction kinetics and spatial selectivity [1-4].

References:

[1] H. Guo, et al., *Nature* **599**, 67-73 (2021).
[2] M.-A. Stoeckel, et al., *Angew. Chem. Int. Ed.* **63**, e202407273 (2024).
[3] W. Jin, et al., *Nature* **630**, 96-101 (2024).
[4] T. Liu, et al., *Nat. Mater.* 10.1038/s41563-026-02547-0 (2026).

Advanced photophysical analysis for elucidating excited-state energy configurations in TADF Materials

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Keywords: Thermally activated delayed fluorescence, Kinetic analysis, Excitonic energy configuration

Since the establishment of molecular design principles for OLED applications in 2011, thermally activated delayed fluorescence (TADF) materials have been extensively developed. Accurate determination of the singlet–triplet energy gap (ΔE_{ST}) is essential for understanding TADF mechanisms and validating quantum chemical calculations. However, experimental estimation of ΔE_{ST} remains challenging because of the limitations of simplified kinetic models and ambiguities in excited-state energy determination, particularly in the near-zero-gap regime.

Here, we demonstrate a comprehensive kinetic analysis based on a dynamic exciton model that provides a higher-resolution description of excited-state configurations than conventional approaches. We investigated two TADF materials, **TMCz-BO** and **HzTFEX2**, which exhibit thermal deactivation in toluene, where delayed fluorescence becomes longer at low temperatures and shorter at high temperatures. Conventional Arrhenius analysis predicts a negative ΔE_{ST} for both materials.

The dynamic exciton model revealed that **TMCz-BO** possesses a positive ΔE_{ST} under all investigated temperature and solvent conditions (Figure 1). In contrast, **HzTFEX$_2$** consistently exhibited a negative ΔE_{ST} under all measured conditions.

In conclusion, the dynamic exciton model enables high-resolution characterization of excitonic state configurations and provides reliable ΔE_{ST} determination in the near-zero-gap regime, overcoming key limitations of conventional Arrhenius-based analyses.

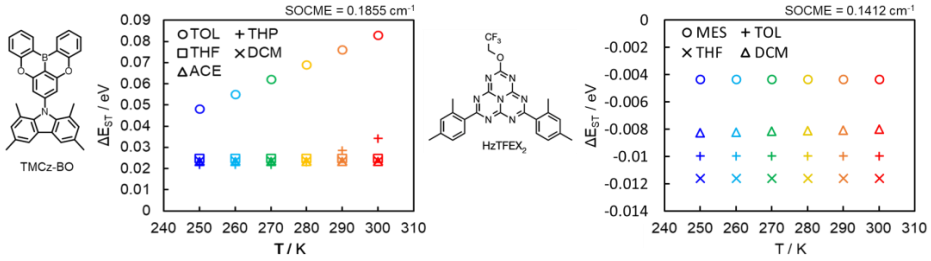


Figure 1: ΔE_{ST} for **TMCz-BO** and **HzTFEX$_2$** estimated by comprehensive kinetic analysis with dynamic exciton model.

References:
[1] Y. Tsuchiya, C. Adachi et al., *J. Phys. Chem. A*, **20**, 45, (2021).
[2] Y. Tsuchiya, C. Adachi, et al., *Nat. Commun.*, **16**, 4815 (2025).
[3] H. Jung, Y. Youichi, C. Adachi, et al., *Appl. Phys. Express*, **19**, 021008 (2026).

Breaking linear scaling relationships in electrocatalytic nitrate reduction to ammonia with high-entropy alloys

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The electrochemical nitrate reduction reaction (NO_3RR) represents a highly promising avenue for sustainable ammonia synthesis. However, its efficiency is severely hindered by complex proton-coupled electron transfer pathways. Furthermore, inherent linear scaling relationships (LSRs) between intermediate adsorption energies create a thermodynamic bottleneck, limiting the simultaneous optimization of successive elementary steps on conventional electrocatalysts. To overcome this thermodynamic limitation, we propose a synergistic strategy utilizing high-entropy alloy (HEA) architectures [1]. Density Functional Theory (DFT) simulations reveal that the intricate interplay of intrinsic lattice strain and multimetallic electronic coupling within the HEA matrix effectively decouples the conventional LSRs. Specifically, the diverse local coordination environments engender synergistic active sites with a tailored strong-medium-weak adsorption energy gradient. This optimized energetic landscape precisely modulates the binding affinities of sequential intermediates across the eight-electron proton-coupled electron transfer pathway, thereby substantially lowering the thermodynamic barrier of the potential-determining step. Using a combination of advanced in situ spectroscopic techniques and electrochemical analysis, we elucidate the evolution of the catalyst surface and identify key reaction intermediates. This study establishes a comprehensive paradigm for designing next-generation high-entropy materials for complex, multi-electron energy conversion processes [2].

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[1] H. Liu and S. Jia, Angew. Chem. Int. Ed. 64, e202510478 (2025)

[2] T. Yang and J. Huang, Chem. Eng. J. 500, 157426 (2024)

Design of thermally activated delayed fluorescence materials for high-performance solution-processed organic light-emitting diodes

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Keywords: TADF, dendrimers, liquid crystals, solution-processed OLEDs

Solution-processed OLEDs (SP-OLEDs) are a potentially attracted alternative to vacuum-deposited devices as they can be fabricated at reduced cost. Device performance has consistently lagged vacuum-deposited OLEDs, even in cases where the emitter is the same. Here, I will present our recent work where we address issues of efficiency, roll-off and color purity by designing next-generation thermally activated delayed fluorescence emitters explicitly conceived to be used in SP-OLEDs.

Generating Fuels from Sunlight Using Polymer Photoelectrodes

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Photoelectrochemical cells made from blends of (printable) conjugated polymers have recently shown promise as platforms that may eventually deliver chemical fuels (e.g. H_2) from sunlight and enable new, broadly accessible pathway to long term energy storage. The ease of optoelectronic tunability in these materials, proven function in high efficiency organic solar cells, and low cost processability make “soft” conjugated polymers fascinating complements to photoelectrochemical platforms based on hard, inorganic semiconductors with surface catalysts. Many current photocathode demonstrations have focused on a protected organic photovoltaic in water, but an alternative approach is to directly submerge the organic semiconductor(s) to drive (photo)catalysis. Controlling polymer/electrolyte interactions in “interphase” regions – a term purposely selected to represent a longer length scale polarization and spatiotemporal behaviors not describable with conventional metal/electrolyte double layer theories - is a long-term goal. These photoelectrochemical systems promise to take greater advantage of the tunability of bandgap, charge generation and charge transport efficiencies, and ease of introduction of catalytic sites into unique micro-environments, but there are significant knowledge gaps that need to be addressed before these materials realize their full potential.

Hybrid thin film materials for sustainable energy devices

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The combination of selected nanostructures to originate hybrid materials allows minimizing limitations of the single compounds, maximizing the intrinsic properties of each one and creating novel and unique properties arising from the synergism coming from the intimate contact between the components at nanometric level. This talk will present a novel and almost unlimited platform to hybrid materials, directly synthesized and processed as thin films, based on interfaces between immiscible liquids [1]. It will present bi- or tri-components materials obtained by the combination of π-conjugated molecules and materials (conducting polymers, carbon nanotubes, graphene) with inorganic materials as MoS_2, copper oxide nanoparticles and Prussian blue analogues, aiming specific application as electrodes to: i) transparent and flexible aqueous sodium- or potassium-ion batteries [2]; ii) aqueous pseudocapacitors and iii) electrochromic devices [3][1]. The evident effect of the nanostructured materials on some superlative properties observed in those electrodes will be demonstrated and discussed based on the structure/properties relationship. For example, specific capacity as high as 1316 mA h g^{-1} for Na-ion aqueous batteries have been found for a MoS_2/Graphene/Cu_2O tri-component nanostructures film, which are among the best results presented in literature for this kind of application. An innovative transparent, flexible, aqueous Na-ion battery full device presenting high stability and performance will be also presented.
Authors acknowledge INCT-NanoVida, INCT-Nanocarbono, CNPq, CAPES.

References
[1] Zarbin, A.J.G.; Mater. Horizons, 8, 409, 2021.
[2] Ramos, M.K.; Zarbin, A.J.G.; Sust. Energy Fuels, 9, 4614, 2025.
[3] Souza, V.H.R.; Schmidt, A.; Zarbin, A.J.G.; J. Mater. Chem. A **11**, 18853, 2023.

Is Polarity Intrinsic? Redefining Charge Transport in Organic Semiconductors through Interfacial Physics

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The conventional classification of organic semiconductors as "p-type" or "n-type" is an oversimplification that overlooks the defining influence of interfacial physics on device behavior. In this presentation, we demonstrate that charge transport polarity is not a fixed material property, but a tunable device property governed by charge injection engineering. We present a universal approach to control the dominant charge carrier in organic field-effect transistors (OFETs) by engineering the charge injection interface to selectively favor either holes or electrons. Validating this strategy, we successfully transformed the archetypal p-type polymer IDTBT into a high-performance n-channel transistor with an electron mobility of 2.3 cm^2/Vs. Conversely, the benchmark n-type polymer N2200 was engineered to operate as an efficient p-channel device. To demonstrate the technological relevance of this principle, we showcase a functional complementary inverter fabricated using a single organic semiconductor layer. This approach drastically simplifies the architecture of organic logic circuits by eliminating the need to pattern discrete p- and n-type channels. These findings establish that transport polarity is determined by device design, allowing sufficiently pure organic semiconductors to be engineered as p-type, n-type, or ambipolar components.

Nanostructured Materials for Chemical Sensing: 2D Nanomaterials and Electrospun Platforms

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Recent advances in nanostructured materials have significantly expanded the possibilities for developing highly sensitive and selective chemical sensing platforms. In particular, two-dimensional (2D) nanomaterials and polymeric nanostructures have emerged as promising building blocks due to their unique electronic, surface, and structural properties. In this talk, recent progress in the development of functional nanostructured materials for chemical sensing will be presented, highlighting two complementary research directions. The first focuses on 2D nanomaterials, including graphene derivatives, graphene quantum dots, and MXenes, which exhibit outstanding electrical conductivity, high surface area, and abundant active sites, all of which are advantageous for sensing applications. The second explores electrospun polymeric nanofibers as versatile platforms for fabricating highly porous materials with tunable morphology and large surface-to-volume ratios. Examples of sensing systems based on these nanostructured materials will be discussed, including strategies for material functionalization, nanocomposite design, and device fabrication. These approaches enable improved sensitivity, fast response, and enhanced interaction with target analytes. Finally, perspectives on the development of next-generation sensing technologies based on nanostructured materials will be addressed, with emphasis on portable and low-cost devices for environmental, agricultural, and biological monitoring.

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Scale-up challenges for third-generation PV | Case comparison for Perovskite- and Organic-PV

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One of the challenges for OPV and Perovskite photovoltaic is finding real solutions for actual and future commercialization. The two photovoltaic technologies, currently under developing at PHD Research, are in a different maturity stage in the applied research and potentially with diversified market prospects by their very nature, at least in the short term. OPV is already a production reality but still with some important challenges such as increasing modules efficiency and their stability for specific applications related a reasonable cost. In the other hand the perovskite PV still needs to do some important steps with, in part, different challenge before being applied commercially. Both technologies require a constant compromise between efficiency, lifetime and costs compatible with the module evolution stage and their final applications. With this talk we will try to understand what potentially join the two technologies and what differentiates them, both from a scale-up point of view.

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References
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Studies of exciton loss processes in OLEDs assisted by kinetic Monte Carlo simulations

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Keywords: OLED, exciton, kinetic Monte Carlo

In contrast to rate equation approaches, kinetic Monte Carlo (kMC) simulations can explicitly account for the molecular-scale quantum effects underlying the functioning of OLEDs. In this work, we use the kMC tool Bumblebee from Software for Chemistry and Materials (SCM) in kMC-assisted studies of exciton loss processes involving field-induced exciton dissociation (FID) in phosphorescent [1] and TADF [2] OLED emission layers, and triplet exciton-polaron quenching (TPQ) in phosphorescent emission layers [3]. In the FID studies, a varying reverse bias voltage leads to bias-dependent dissociation of photogenerated excitons, which can be quantified by measuring the photocurrent and the photoluminescence (PL) efficiency as a function of bias voltage. From a fit to kMC results we can determine the exciton binding energy, which is found to be in the range 1.0-1.3 eV for the studied phosphorescent emitters and 0.8-1.3 eV for the studied TADF emitters. In the TPQ studies, the temperature-dependent current density-voltage characteristics of single-carrier carrier devices are first measured and modeled with kMC simulations, so that the polaron density as a function of current density is known. Subsequently, the current density-dependence of the steady-state and time-resolved PL spectra is measured and fitted with kMC simulations, also taking into account FID. From the optimal fits we can determine the Förster radius for the TPQ process, which is found to be in the range 3.5-5.5 nm for triplet-hole polaron quenching in the studied emitter-host combinations. Our studies demonstrate the power of kMC simulations in describing complex exciton loss processes in OLEDs and thus their potential to assist in the design of OLEDs with improved efficiency.

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References:
[1] H. Tomita, L.R.L. Norg, P. Diederen, C. van Hoesel, C.H.L. Weijtens, P.A. Bobbert, and R. Coehoorn, Advanced Functional Materials (2026) 0:e75896.
[2] H. Tomita, C.B. McDonald, C. van Hoesel, C.H.L. Weijtens, P.A. Bobbert, and R. Coehoorn, to be published.
[3] H. Tomita, C. van Hoesel, C.H.L. Weijtens, P. A. Bobbert, and R. Coehoorn, to be published.

Sub-microsecond Delayed Fluorescence Enabled by Molecular Engineering of Triazatruxene Emitters for High-Performance OLEDs with Suppressed Efficiency Roll-off

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Keywords: Thermally activated delayed fluorescence (TADF), organic light emitting diodes (OLEDs), triazatruxene (TAT), sub-microsecond delayed lifetime, efficiency roll-off

Purely organic thermally activated delayed fluorescence organic light emitting diodes usually suffer from strong efficiency roll-off, defined as the decrease in external quantum efficiency at high luminance. One of the primary causes of this roll-off is the long excited-state lifetime and slow reverse intersystem crossing process of emitters. In this work, we designed a series of donor-acceptor-type TADF emitters TAT-(4BPy), TAT-2(4BPy), and TAT-3(4BPy) by gradually increasing the acceptor substitution around a central triazatruxene donor. Both, theoretical and photophysical studies showed a gradual blue shift of the absorption and emission while moving from TAT-(4BPy) to TAT-3(4BPy). Increasing acceptor substitution resulted higher percentage of locally excited character in the triplet state, resulted in a progressively shorter excited state lifetime, faster rISC rate, and better spin-orbit coupling. Doped film of the emitters displayed sub-microsecond time scale delayed fluorescence (DF), specifically TAT-3(4BPy) showed the shortest lifetime among all and a fastest k_{rISC} of 9.61 x 10^5 s^{-1}. PLQY and krISC follow opposite trend. The EQEs of TAT-(4BPy), TAT-2(4BPy), and TAT-3(4BPy) based OLEDs were 29.1%, 24.6%, and 20.0%, respectively. Among the three devices, TAT-2(4BPy) demonstrates the lowest efficiency roll-off of only 6.5% and maintains an EQE of 23.0% at 1000 cd/m^2. As per the conventional understanding, TAT-3(4BPy) should exhibit the lowest roll-off, due to its fastest k_{rISC}. However, our findings reveal that both a faster rISC and a comparatively smaller DF contribution collectively help in getting minimum efficiency roll-off.

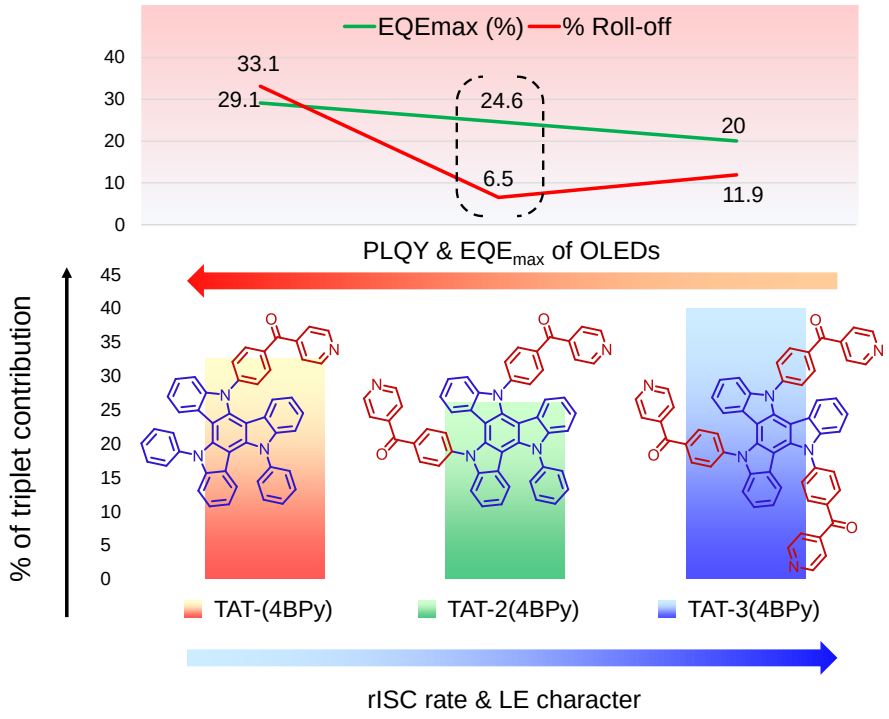


Figure 1: Three emitters with gradually increased acceptor substitution were developed. With increasing acceptor number, the PLQY decreases, while the rISC rate increases. The middle emitter provides the optimal balance between these competing factors, enabling OLED with the highest external quantum efficiency and the lowest efficiency roll-off.

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References:

[1] G. P. Nanda, R. Suraksha, P. Rajamalli, ACS Materials Au, 604 (2024).
[2] G. P. Nanda, R. Suraksha, B. Sk, T. Viswanathan, P. Rajamalli, Journal of Materials Chemistry C, 14953 (2025).
[3] U. Deori, E. Ravindran, G. P. Nanda et al., Chemistry – An Asian Journal, e202300352 (2023).

Towards a conformable, sustainable and multifunctional organic field-effect transistor platform

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Keywords: OFET, OLET, conformable, sustainable

The combination of organic and hybrid nanomaterials as functional layers of field-effect device architectures enables the development of devices for a variety of applications, including electronic sensing, light generation and cell interfacing. We discuss the concept of Organic Light-Emitting Transistors (OLETs), highlight their specific electrical, optoelectronic and photonic characteristics, and of transparent silicon-free transistor structures that are biocompatible and provide bidirectional stimulation and recording of neural cells. Here we address the limiting factors of rigidity and sustainability of multifunctional field-effect devices by investigating flexible and conformable substrates as well as sustainable hybrid dielectrics. Attention will be given to the correlation between surface engineering, morphology of the field-effect functional layers and electrical/optoelectronic characteristics under flat and bent measuring conditions.

Vertical Organic Electrochemical Transistors and Neuromorphic Devices

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Vertical Organic Electrochemical Transistors (vOECTs) have recently emerged as a novel platform in organic electronics, enabling high performance through ultrashort channel lengths achieved via a perpendicular channel architecture. This geometry enables high transconductance, fast response times, and exceptional sensitivity to ionic and redox stimuli.
In this work, we present a comprehensive analysis of the scaling laws governing vOECTs and derive design rules to further optimize their performance. We demonstrate how the inherently high transconductance enables intrinsic signal amplification of minute chemical changes, leading to exceptional sensitivity—making vOECTs ideal for next-generation biosensors and environmental monitors.
Our vOECT design features a channel formed by electropolymerization of an organic semiconductor between stacked source and drain electrodes, separated by a thin insulating layer. Crucially, we demonstrate that the electrical connection between source and drain can be modulated by applying short voltage pulses to the gate, allowing precise control over the polymerization extent and thus the channel conductivity. This enables the fabrication of reconfigurable, neuromorphic devices and circuits with tunable synaptic behavior. By leveraging this programmable electrochemical process, we establish a hardware-based foundation for artificial neural networks, paving the way for energy-efficient, in-situ computing systems integrated with biological interfaces.

Wafer-scale organic single crystals: integrated circuits and quantum charge transport

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Keywords: organic semiconductor, organic single crystal wafer, analogue/digital integrated circuits, metal insulator transition, strong electron correlation, quantum oscillation

Recent development of organic semiconductors presents significant progress in small-molecular crystals, achieving high carrier mobility based on coherent electronic transport. Extremely thin crystal films of Cn-DNBDT small molecules are successfully grown to a-few molecular layers with the thickness of only 10 nm, so that very high carrier mobility more than 10 cm^2/Vs is achieved to the dimension of 30 cm x 30 cm [1]. Single crystal field-effect transistors of such materials display coherent band transport near room temperature as the result of Hall-effect measurement. The cut-off frequency reaches as high as 75 MHz so that small-scale integrated circuits are practically meaningful [2].

Current technologies for printed integrated circuits provide a manufacturable process for low-cost platforms for RFID tags, sensing circuitries, and large-area light-weight display sheets. Digital circuits of 3-stage shift resistors are fabricated with the newly developed solution processed organic single-crystalline p-type semiconductors and inorganic amorphous n-type semiconductors. The channel length is typically 4 μm so that nearly 100 transistors are integrated in the area of approximately 5 mm^2. The circuit shows the proper resistor function at the maximum frequency of 12 kHz. Analogue circuits of differential amplifiers are also fabricated by the same process. The amplifier is operated with the excellent gain-bandwidth (GB) product of as high as 1,000,000, which are both the best values ever reported for solution processed flexible circuits. With excellent chemical and thermal stability of the materials, the established organic-inorganic hybrid CMOS processing technologies realize practical integrated circuits on flexible films.

Employing the molecule composed of an elongated π-electron core and σ-electron units connected to both edges of the core, a quantum well is formed as the result of two-dimensional crystallization. We attach a electron-accepting layer on the surface of the ultrathin molecular crystals without modifying the crystal structure. Upon doping with an electric double-layer gate of an ionic liquid, the 2D crystal layer of the π-electron core is well protected from invasion of the anions, so that high carrier mobility exceeding 20 cm^2/Vs is preserved with 1/4 holes per molecule, resulting in the first observation of metallic phase in organic semiconductors [3]. At the high carrier concentration of about 10^{14} cm^{-2}, which approximately fills 1/8 of the HOMO band, a pseudo-gap phase appears as the result of strong electron correlation.

References:

[1] C. Mitsui, T. Okamoto, J. Takeya et al., Adv. Mater. 26, 4514 (2014).
[2] T. Sawada, S. Watanabe, J. Takeya et al., Nature Commun. 11, 4839 (2020).
[3] Kasuya, N.; Watanabe, S.; Takeya, J. et.al. Nature Mater. 20, 1401 (2021).

A photo-patternable solid-state electrolyte for high-performance, miniaturized, and implantable organic electrochemical transistor-based circuits

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Organic electrochemical transistors (OECTs) represent a rapidly advancing technology that plays a pivotal role in the development of next-generation bioelectronic devices. However, a notable limitation of OECTs is their typical operation in aqueous electrolytes, which can lead to undesired crosstalk between different devices on the same substrate, impeding their seamless integration into large-area arrays. Here, we reported the design of □-CGN-based hydrogel electrolytes for solid-state OECTs. These hydrogels can be directly photopatterned down to 15 µm, enabling the processing of large-area solid-state OECTs with electrical performance (e.g., transconductance and switching speed) on par with aqueous electrolytes. We demonstrate compact solid-state NAND/NOR gates (500×800 µm2), 4-input NAND gates (1600×800 µm2, 8 OECTs), and half-adders (2×1 mm2, 18 OECTs), all exhibiting correct logic functions and low-voltage operation. To highlight its potential for implantable bioelectronics, we developed solid-state spiking circuits, monolithically integrated with flexible cuff electrodes, for vagus nerve stimulation in mice. These findings establish □-CGN-based solid-state electrolytes as a promising platform for scalable, implantable circuits, paving the way for next-generation bioelectronic devices.

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References
Adv. Mater. 2025, 37, e09314

Nat. Mater. 2023, 22, 242.

Advancing the Scale-Up of Third-Generation Photovoltaic Devices: Deposition Process Stability, Repeatability, and Reproducibility

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Third-generation solar cells have experienced remarkable advancements in recent years, achieving record-breaking power conversion efficiencies (PCE) in small-area devices. Despite this progress, the NLR-certified PCE values for large-area photovoltaic modules, including organic photovoltaics (OPVs) and perovskite-based devices (PSC), remain significantly lower, highlighting a critical lab-to-fab technological gap between laboratory-scale performance and industrial-scale applications.

In this context, the present work provides a comprehensive analysis of the main advances, challenges, and strategies associated with scaling up the production of third-generation photovoltaic devices. Initially, the critical factors governing operational stability and rigorous process control are discussed, with particular emphasis on key parameters such as repeatability, reproducibility, and production yield, considering the current maturity level of (OPVs) and (PSCs).

Furthermore, the analysis spans multiple scales, ranging from small-area devices (~0.55 cm^2) to commercially scaled OPV modules exceeding 6000 cm^2, as well as the development of the first perovskite photovoltaic panel in Brazil, achieved through the interconnection of mini-modules in series and parallel, resulting in a device measuring 27 cm × 33 cm with an active area of 483 cm^2.

Finally, this work highlights the fundamental requirements for the effective transition of these technologies from the laboratory environment to pilot production and, ultimately, to large-scale manufacturing.

References

Shah, N.; Shah, A.A.; Leung, P.K.; Khan, S.; Sun, K.; Zhu, X.; Liao, Q. A Review of Third Generation Solar Cells. Processes 2023, 11, 1852. https://doi.org/10.3390/pr11061852

NATIONAL RENEWABLE ENERGY LABORATORY (NREL). Champion Photovoltaic Module Efficiency Chart. Disponível em: . Acesso em: 31 mar. 2026.

Air-Processed Inverted PM6:Y6 Solar Cells on Glass/FTO

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Inverted organic solar cells based on the PM6:Y6 blend were fabricated under ambient conditions on glass/FTO substrates using the architecture FTO/ZnO/active layer/MoO_3/Ag. The devices reached a power conversion efficiency of ~16%, demonstrating efficient operation under air processing on rigid transparent electrodes. Spectroscopic ellipsometry was employed to characterize the complete multilayer stack, enabling simultaneous determination of thickness and optical constants of the individual layers within the device architecture. The extracted optical parameters revealed well-defined absorption features across the heterostructure, including signatures consistent with favorable molecular packing and electronic coupling between components. The consistency of the fitted optical models indicates controlled film formation and reproducible interface definition under ambient conditions. The correlation between ellipsometric parameters of the full stack and the electrical characteristics establishes a comprehensive structure–optical–device relationship in air-processed PM6:Y6 systems. The implementation on glass/FTO substrates, compatible with transparent conducting architectures, reinforces the technological relevance of these findings for scalable organic photovoltaic platforms on rigid transparent substrates.

References

RASOOL, Shafket; KIM, Jin Young. Prospects of glove-box versus air-processed organic solar cells. Physical Chemistry Chemical Physics, v. 25, n. 29, p. 19337-19357, 2023.

An analytical model for antiambipolar organic electrochemical transistors

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Antiambipolar Organic Electrochemical Transistors (OECTs) exhibit a bell-shaped transfer characteristic in which the drain current increases to a maximum and then decreases with further gate voltage increase. This behavior gives rise to negative differential resistance (NDR), a property highly relevant for nonlinear and neuromorphic circuits. Although the phenomenon has been explored experimentally, a predictive analytical model has been lacking, and existing OECT models fail to capture antiambipolarity or provide physical insight into its origin. Here, we introduce the first analytical framework that quantitatively describes antiambipolar OECTs, establishing a direct link between electrochemical redox processes and transistor-level current–voltage characteristics. Based on the electrochemical properties of the reference antiambipolar polymer BBL and building on our previously reported electrochemical framework[1], we derive an analytical expression that accurately predicts and fits the experimental current–voltage behavior. Although demonstrated using BBL, the framework is general and applies to electrochemical semiconductors exhibiting multi-step redox processes. Our model shows that antiambipolarity arises from a trade-off between singly and doubly charged species. The first redox process generates mobile singly charged carriers, while a second redox process forms immobile doubly charged species that reduce the density of mobile carriers. This interplay produces the characteristic bell-shaped transfer curve. Additionally, we derive an analytical expression for the gate voltage corresponding to the peak drain current as a function of device and electrolyte parameters, a key quantity for circuit design using single-device NDR elements. This work provides a theoretical foundation for controlling and optimizing antiambipolar OECTs for advanced electronic applications.

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References

B de A., Feitosa, et al., Materials Horizons, 6007-6018, 11 (2024).

Charge Carrier Transport and Trap Levels on Solution-Processed Zn(II) Schiff Bases OLEDs

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Organic light-emitting diodes (OLEDs) are a leading display technology, yet achieving high efficiency in first-class fluorescent OLEDs remains a challenge due to limited internal quantum efficiency (IQE) [1,2]. In this study, we report a comprehensive investigation of Zn(II) Schiff base coordination compounds as first-class fluorescent emitters embedded in solution-processed active layers based on poly(9,9′-dioctylfluorene) (PFO). To enhance charge-carrier balance and device performance, two strategies were employed: (i) introduction of a TPBi electron-transport layer (ETL) and (ii) incorporation of the n-type material OXD-7 into the PFO matrix, forming an exciplex host. Devices fabricated from both room-temperature and hot solutions were characterized. Electroluminescence spectra revealed near-white emission due to efficient energy transfer between the host and guest materials. Charge-transport analysis using space-charge limited current (SCLC) models [3] revealed that hot processing increases trap densities (NT), while OXD-7 incorporation reduces NT under cold processing. Among the emitters, Zn(BTS) and Zn(sal-3,4-ben) showed the highest device efficiencies in PFO and PFO:OXD-7 matrices, respectively, achieving current efficiencies up to 10.48 cd A^{-1} and EQEs exceeding 6%. The results demonstrate improved charge balance and reduced roll-off behavior, linking electrical and optical properties through quantitative trap-state analysis and electronic mobility estimations. This study provides a route to high-performance, cost-effective near-white OLEDs based on Earth-abundant Zn(II) coordination complexes.

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References

C. W. Tang and S. A. Vanslyke, Appl. Phys. Lett., 1987, 51, 913–915.

J. Eccher, W. Zajaczkowski, G. C. Faria, H. Bock, H. von Seggern, W. Pisula and I. H. Bechtold, ACS Appl. Mater. Interfaces, 2015, 7, 16374–16381.

E. S. Moraes, L. G. T. A. Duarte, F. S. Rodembusch, J. C. Germino, L. F. R. Pereira and T. D. Z. Atvars, Mater. Adv., 2024, 5, 7778–7788.

Charge Transport and Doping Physics in Mixed Lead–Tin Perovskites

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Mixed lead–tin halide perovskites is a powerful material platform for investigating how band structure, defect chemistry, and doping influence charge transport in soft semiconductors. However, measurement of their bulk transport properties remains challenging due to the material's poor ambient stability. This study presents a systematic and thorough investigation uncovering the doping landscape and charge transport mechanisms from lead-rich to tin-rich triiodide perovskite compositions.

We first developed a robust patterning and encapsulation workflow to fabricate perovskite Hall bars for Hall-effect and thermoelectric measurements. By varying the Pb–Sn ratio from lead-rich to tin-rich, hole densities ranging from 10^{15} to 10^{19} cm^{-3} and mobilities were accurately measured using a homemade, high-accuracy Hall-effect setup. Through temperature-dependent measurements of the mobility-temperature relation, the transition of charge transport mechanisms—from acoustic phonon scattering and impurity scattering to hopping—is shown to be strongly correlated with composition and hole concentration. On-chip thermoelectric measurements also reveal a change in the hole effective mass due to the mixing of lead and tin. This work establishes a robust methodological framework and a comprehensive transport physics map for understanding and optimizing narrow-bandgap perovskites for future optoelectronic applications.

Acknowledgements
EP/Z531303/1, EP/W017091/1

References
https://www.repository.cam.ac.uk/items/31327a3b-d54c-4e0f-98f7-69712d638426

Comparative Study of Organic and Inorganic Electron Transport Layers for Organic Solar Cells

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Organic solar cells (OSCs) have been the focus of attention for many researchers around the world due to the development of new non-fullerene acceptor (NFA) materials and their derivatives, achieving conversion efficiencies above 18.5% in small devices (Gao et al., 2025) and over 14% in large-area devices (Basu et al., 2024). The electron transport layer (ETL) is a key part of the structure and has the function of transporting electrons from active material to the cathode layer (ITO), reducing charge recombination losses (blocking holes). Furthermore, this layer in specifically helps to improve the electrical efficiency of the device through the alignment of energy levels at the interface, also contributing to a better morphology and stability. Organic ETL's have advantages such as solution processability, tunable electronic properties and easy compatibility with flexible substrates (Abubaker, 2024). As a counterpoint, this kind of solution suffers from poor stability (Al-ahmad et al., 2022). Inorganic's ETLs, on the other hand, present superior chemical robustness, higher electron mobility, and improved long-term stability, though they may require more complex processing conditions (Lee et al., 2025) This study consists on the evaluation of both types of materials (organic-based / inorganic-based) through a slot-die roll-to-roll (R2R) process, focusing on the parameters such as power conversion efficiency (PCE), fill factor (FF), short-circuit current density (Jsc), series resistance (Rs) and stability. The results highlight the trade-offs between processability and durability, providing insights into the selection and optimization of ETL materials for next-generation organic photovoltaic devices. The samples for these experiments were produced by using a R2R process with slot die coating inside of the PHD Research Center in Belo Horizonte, Brazil. The results will show the main differences in the use of the two different types of ETL at a pre-industrial scale.

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References

S. A. Abubaker, M. Z. Pakhuruddin, Energy Technology, (2024).

A. Al-Ahmad, et al., Coatings, 12, 1071 (2022).

J. Lee, et al., Applied Physics A, (2025).

Compositional Self-Doping in FA/Cs Perovskites for All-Perovskite Homojunction Solar Cells

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Perovskite solar cells have emerged as a promising photovoltaic technology due to their increase in power conversion efficiency [1]. Among the strategies explored to enhance performance, interface optimization remains one of the most investigated approaches. In this context, perovskite-perovskite homojunctions offer an attractive route by exploiting compositional self-doping [2], where the electronic character is tuned by stoichiometry without extrinsic dopants. Combining p-type, intrinsic, and n-type regions within the same material family promotes selective charge extraction while limiting heterogeneous interfaces. Here, we studied thermally co-evaporated FA/Cs lead iodide perovskite films with controlled precursor ratios to tune their doping character and assess their use in all-perovskite homojunction solar cells. Using ultraviolet photoelectron spectroscopy and inverse photoelectron spectroscopy, we analyzed the valence and conduction band edges as a function of composition. The relative amount of iodide precursors modified the Fermi level within the bandgap, enabling a continuous transition from n-type to p-type behavior while preserving the same perovskite family. These measurements confirmed that self-doping remains operative in mixed FA/Cs systems and can guide junction design. Based on these results, homojunction solar cells were fabricated by combining perovskite layers with different doping character in a p-i-n configuration. Compared with reference devices, the best architecture showed a 2.5-fold increase in power conversion efficiency and a twofold increase in short-circuit current density. This improvement was associated with more efficient charge extraction and transport, enabled by doped perovskite regions while maintaining an intrinsic absorber. Overall, this work shows that spectroscopically guided compositional control is effective for all-perovskite homojunctions and supports the development of simplified perovskite device architectures.

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References

NREL. Best Research-Cell Efficiency Chart. 2026; Available from: https://www.nrel.gov/pv/assets/pdfs/best-research-cell-efficiencies.pdf.

Paul, G., et al., Self-Doping in Hybrid Halide Perovskites via Precursor Stoichiometry: To Probe the Type of Conductivity through Scanning Tunneling Spectroscopy. The Journal of Physical Chemistry C, 2018. 122(35): p. 20194-20199.

Contact resistance dependence on the surface-functionalization time in bottom-contact organic thin-film transistors

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Contact resistance is a significant constraint in organic thin-film transistors (TFTs), becoming increasingly detrimental to device performance as the channel lengths are reduced. In p-channel organic TFTs employing the inverted coplanar (bottom-contact) device architecture, functionalization of the surface of the metal source and drain contacts with a chemisorbed pentafluorobenzenethiol (PFBT) monolayer has been shown to reduce the contact resistance [1]. A large number of fabrication protocols employing different solvents, concentrations, and functionalization times have been reported for such thiol-based contact treatments. Although these fabrication parameters are known to influence monolayer formation [2], their direct impact on contact resistance in bottom-contact TFTs has rarely been the subject of a systematic study. Here we examine the influence of the functionalization time (duration of immersing the substrate into the PFBT solution) on the electrical performance of bottom-contact TFTs based on the small-molecule semiconductor 2,9-diphenyl-dinaphtho[2,3-b:2′,3′-f]thieno[3,2-b]thiophene (DPh-DNTT). A pronounced dependence of the contact resistance on the functionalization time is observed: TFTs whose contacts were immersed into a PFBT solution for 30 s exhibit nearly a threefold lower contact resistance (as small as 39 Ωcm) than devices immersed for 3 hours. In addition to a low contact resistance, the TFTs have an intrinsic channel mobility of 4.2 cm^2/Vs, a subthreshold swing of 82 mV/dec and an on/off current ratio of 10^(7). Surface characterization using Kelvin probe force microscopy, cyclic voltammetry, and X-ray photoelectron spectroscopy revealed an increase in molecular coverage and surface-potential uniformity with increasing exposure time. These results highlight the sensitivity of device performance to contact functionalization parameters and emphasize the importance of carefully controlling fabrication parameters in organic TFTs.

References

Borchert, J. W., et al., Advanced Materials, 34, 2104075 (2022).

Love, J. C., et al., Chemical Reviews, 105, 1103–1169 (2005).

Critical Assessment of Mobility and Contact Resistance in Metal Halide Perovskite Field-Effect Transistors

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Field-effect mobilities as high as 20–80 $cm^2 V^{-1} s^{-1}$ have been reported in metal halide perovskite transistors. These values has raised concerns because device non-idealities and contact resistance can distort mobility extraction. In organic semiconductors, such issues are commonly addressed using gated four-point-probe (4PP) FET measurements, yet this method has not been applied to recent high-mobility reports in tin perovskites.

Here we performed gated 4PP FET measurements on patterned Hall-bar devices based on $Cs_{0.15}FA_{0.85}SnI_3$ and obtained a 4PP mobility of 3.3 $cm^2 V^{-1} s^{-1}$. On the same chip, a narrow-channel (L/W = 0.1) 2P FET showed a strong dependence of extracted mobility on both V_{DS} and V_G. By directly extracting the contact resistance (R_C) from the 4PP data, we found that R_C is significantly modulated by both voltages. Low V_{DS} causes underestimation of linear 2P mobility due to the voltage drop across R_C, whereas high V_{DS} leads to overestimation in saturation because of a large derivative of R_C to V_G. Our work shows that gated 4PP method is the most effective approach to eliminate the influence of contact resistance in mobility extraction and probe the clean charge transport properties in FETs. We therefore recommend that future reports of high FET mobilities (>10 $cm^2 V^{-1} s^{-1}$) in metal halide perovskites and other novel semiconductor material systems include 4PP FET data. Saturation regime 2P mobility is the least reliable as it often leasts to significant overestimation of mobility values.

For additional methodological highlights, we showed that perovskite films can be easily patterned by mechanical scratching or rubbing, allowing straightforward fabrication of Hall-bar patterns for 4PP measurements. For mobility extraction methodologies, we revisited the original silicon MOSFET model and proposed rigorous methods and proposed rigorous methods and criteria to extract V_G-dependent mobilty and R_C in 4PP measurements.

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References
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Cross-linked naphthalene diimide small molecules as multifunctional electron transport layers for perovskite solar cells

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Electron transport layers (ETLs) are key components in perovskite solar cells (PSCs). Beyond extracting and transporting electrons from the perovskite absorber, ETLs can also improve device stability by passivating interfacial defects, reducing non-radiative recombination, and mitigating degradation pathways. This expanded role motivates the development of multifunctional, colorless ETLs that combine efficient charge extraction, fast electron transport, and interfacial protection [1]. However, designing organic ETLs that meet these requirements remains challenging, particularly when incorporating self-doping motifs to enhance conductivity and crosslinkable groups to improve film robustness, solvent resistance, and long-term operational stability. In this oral presentation, we report our first results using a naphthalene diimide (NDI)-based small-molecule ETL in p–i–n PSCs employing a triple-cation perovskite absorber. Preliminary investigations showed that devices incorporating the NDI ETL reached a power conversion efficiency (PCE) of 7%. While the initial performance remains below the fullerene benchmark, these results validate NDI derivatives as solution-processable ETLs and provide a foundation for further molecular and interfacial optimization. We also present the complete synthesis of a next-generation NDI platform combining easy crosslinking and self-doping functionalities, designed to strengthen interfacial durability, protect the perovskite from moisture, and enhance electron transport. Importantly, these molecules are highly stable, straightforward to prepare, and colorless, making them promising candidates for tandem PSCs where minimal parasitic absorption is required. Additional optimization and device results will be discussed.

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References
Y. Bai et al., Nat. Commun. 7, 12806 (2016)

Design of photonic electrophoretic devices based on hybrid silica-polymer colloids

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Electrophoretic colloidal crystals (ECC), discovered by Shim et al. in 2010, are self-assembled arrays of charged colloidal particles whose photonic bandgap can be dynamically tuned by an applied electric field [1]. This ultra-low-power technology holds great potential for applications in smart insulation, camouflage, reflective displays, and anticounterfeiting technologies. While polar ECC are now relatively well understood structurally, their apolar counterparts, essential for industrial electrophoretic devices requirements, remain almost entirely uncharacterized at the structural level [2]. The central challenge lies in the absence of the electrostatic repulsion ubiquitous in polar media, making both particle charging and colloidal assembly far more difficult [3]. We recently developed a novel approach to prepare apolar ECC based on hybrid hairy particles. Using a straightforward graft-through polymerization technique, monodisperse silica particles were sterically stabilized in apolar media. These particles were successfully self-assembled into photonic structures displaying bright structural colors. However, preliminary results revealed insufficient sensitivity to electric fields, likely due to a lack of surface charge. To address this, the grafted polymer chemistry was investigated to elucidate the relationship between surface chemistry and particle charging, using zeta potential measurements as a function of surfactant concentration and polymer composition. Finally, drawing inspiration from Panther Chameleons, the incorporation of a melanin-like light-absorbing layer was explored to broaden the accessible color gamut and enhance the visual contrast of the photonic structures.

References

Shim, T. S.; Kim, S.; Sim, J. Y.; Lim, J.; Yang, S. Advanced Materials 2010, 22 (40), 4494–449

Bao, Q.; Braun, S.; Wang, C.; Liu, X.; Fahlman, M. Advanced Materials Interfaces 2019, 6 (1), 1800897

Espinosa, C. E.; Guo, Q.; Singh, V.; Behrens, S. H. Langmuir 2010, 26 (22), 16941–16948

Design rules to minimize the non-radiative voltage loss in organic solar cells

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Reducing voltage losses is essential for advancing the efficiency of organic solar cells (OSCs), yet state-of-the-art non-fullerene acceptors (NFAs) still exhibit substantially larger non-radiative losses than their inorganic counterparts.1 Here, we identify intermolecular interaction as a key intrinsic factor limiting radiative recombination in Y-series NFAs. Using an oligomer-based model strategy, we demonstrate that the intermolecular interaction, strongly hybridized with the local exciton, suppresses the radiative decay rate by reducing the oscillator strength of the lowest excited state. This hybridization leads to a diminished photoluminescence quantum yield (PLQY) and prolonged emission lifetimes, consistent with the emergence of partially dark excitonic states. Guided by this mechanistic insight, we develop a molecular design strategy based on side-to-tail coupling to promote J-type excitonic interactions. Devices employing this design achieve a non-radiative voltage loss as low as 0.13 eV, among the lowest reported for OSCs to date. These results establish controlled excitonic coupling as a powerful design principle for minimizing voltage losses and advancing next-generation high-efficiency OSCs.

References

Nakul Jain et. al. Adv. Energy Mater. 2026, 16, 24036.75.

Designing a Carbon Nanotubes/MoS_2/Prussian Blue Three-Component Nanoarchitecture for Superior Aqueous Potassium-Ion Storage

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Aqueous batteries have been studied and developed over the past decades as safer, lower-cost and more sustainable alternatives to conventional lithium batteries [1,2]. In this context, this work describes the synthesis, characterization, and application of a novel three-component nanoarchitecture composed of carbon nanotubes (CNTs), molybdenum disulfide (MoS_2), and Prussian Blue (PB), developed to act as a cathode material for aqueous potassium-ion batteries. Thin films of CNTs and MoS_2 were initially prepared via the liquid–liquid interfacial route (LLIR) and employed as precursors for the electrosynthesis of PB. The electrochemical deposition was systematically investigated by varying the pH of the medium, the applied potential window and the number of electrodeposition cycles to optimize the growth conditions of PB on the precursor material. The obtained samples were characterized by UV–Vis and Raman spectroscopy, scanning electron microscopy (SEM) and different electrochemical techniques. The results confirmed the successful formation of the three-component material, evidencing intimate contact among its constituents. The incorporation of MoS_2 promoted significant differences compared to the control films (without MoS_2), inducing preferential PB growth over the MoS_2 flakes. This effect enabled the electrosynthesis of PB under pH and potential window conditions previously unfavorable for its growth in the bicomponent films. As a consequence, the three-component composite exhibited enhanced electrochemical stability over consecutive cyclic voltammetry cycles, with an 11% increase in current retention compared to the control material. Galvanostatic charge–discharge tests revealed typical battery behavior for all three-component samples. The optimized sample achieved a specific capacity of 160 mAh g^{-1} in 0.5 mol L^{-1} KCl solution within a potential window of 0.0–0.6 V, representing a 28% improvement compared to its control film.

Acknowledgements
CAPES, CNPq, INCT-Nanovida and INCT-Nanocarbono

References

[1] M. K. Ramos; A. J. G. Zarbin, Sustainable Energy & Fuels, v. 9, n. 17, p. 4614-4627 (2025)

[2] S. Husmann; A. J. G. Zarbin; R. A. W. Dryfe, Electrochimica Acta, v. 349, p. 136243 (2020)

Edible Organic Electrochemical Transistor for pH Sensing: Gate-Driven Mechanism and Device Physics

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Monitoring pH variations along the gastrointestinal (GI) tract is essential for diagnosing and managing disorders such as acid reflux, peptic ulcers, and inflammatory bowel disease [1]. Conventional methods, including endoscopy and catheter-based pH probes, are invasive and unsuitable for continuous monitoring. Ingestible electronic systems provide an alternative; however, they often integrate rigid components, batteries, and encapsulation layers that are only partially biocompatible and fail to degrade entirely within the gastrointestinal tract. [2] This incomplete degradation can lead to potential risks such as obstruction or necessitate retrieval procedures. In contrast, an edible system ensures both safety and complete biodegradability, eliminating the need for extraction and avoiding e-waste. Here, we present an edible platform for pH sensing based on an organic electrochemical transistor (OECT). The device integrates inkjet-printed gold source and drain electrodes transferred onto an ethyl cellulose substrate, with Copper(II) phthalocyanine (CuPc) as the semiconductor. Operation in aqueous electrolyte is achieved using a coiled platinum gate electrode. The transistor was characterized in buffer solutions spanning pH 2–11, covering the dynamic range typically encountered along the GI tract. Transfer curves exhibit systematic threshold-voltage (V_th) shifts with a sensitivity of ~50 mV/pH under low-voltage operation (<1 V). Reference-gated measurements using Ag/AgCl demonstrate that the CuPc channel is intrinsically insensitive to pH within the investigated V_GS window (−0.6 to 0.1 V). Independent open-circuit potential measurements reveal that the pH response originates from electrochemical potential shifts at the gate–electrolyte interface. This work introduces a new class of edible, low-power transistors for real-time pH monitoring inside the body, and lays the groundwork for next-generation ingestible diagnostics and fully transient biomedical systems.

References

A. S. Sharova, F. Melloni, G. Lanzani, C. J. Bettinger, and M. Caironi, “Edible Electronics: The Vision and the Challenge,” Adv Mater Technol, vol. 6, no. 2, p. 2000757, Feb. 2021, doi: https://doi.org/10.1002/admt.202000757.

C. Cheng et al., “A wireless, ingestible pH sensing capsule system based on iridium oxide for monitoring gastrointestinal health,” Sens Actuators B Chem, vol. 349, p. 130781, 2021, doi: https://doi.org/10.1016/j.snb.2021.130781.

Effect of Copper Particle Morphology on Conductive COC Composites for 3D Printing

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The integration of additive manufacturing with functional electronic materials enables new opportunities for rapid prototyping of customized electronic components. In this work, we report highly filled conductive composites based on cyclic olefin copolymer (COC) and copper particles for fused filament fabrication (FFF) 3D printing. COC was selected due to its low dielectric loss, chemical resistance, and high thermal stability, making it suitable for electronic applications. A key advancement is the successful incorporation of up to 76 wt% copper into the COC matrix, which is unusually high for thermoplastic composites while maintaining printability. Two copper particle morphologies, dendritic and flake shaped, were systematically investigated to evaluate their influence on rheological behavior, filler networking, and electrical conductivity. A strong morphology dependence of electrical percolation was observed. Composites filled with dendritic copper particles exhibited electrical conductivity due to the formation of interconnected conductive pathways, which was confirmed by a measured resistance of 2.04 Ω in filament. In contrast, systems based on flake shaped and spherical copper particles remained electrically insulating even at high filler loadings, indicating insufficient network formation despite comparable overall composition. Despite the high copper content, the composites retain the inherent thermal stability of the polymer, with a decomposition temperature T_{95} remaining at approximately 440 °C. The developed COC copper composites demonstrate that particle morphology is a critical design parameter governing percolation and electrical performance in highly filled polymer systems. These materials offer a promising route toward 3D-printed conductive elements for advanced electronic and hybrid applications.

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References

X. Zhou, L. Wu, J. Wang, Composites Part A: Applied Science and Manufacturing, 174, 107739 (2023).

D. Pejak Simunec, A. Sola, Advanced Engineering Materials, 24, 2101476 (2022).

Electroluminescent photoresist enabling sub-diffraction nanopatterning of full-color OLED displays

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The miniaturization of organic light-emitting diodes (OLEDs) is critical for next-generation ultrahigh-resolution displays and integrated photonics. However, traditional vacuum evaporation and inkjet printing methods are incompatible with the lithographic scaling processes that underpin silicon electronics, hindering true monolithic integration with complementary metal-oxide-semiconductor (CMOS) circuits. Here, we present electroluminescent photoresists (ELPRs) synthesized via atom transfer radical polymerization that can be directly patterned by ultraviolet (UV) and electron beam lithography (EBL). These multi-arm star polymers feature a core-shell architecture designed to embed the thermally activated delayed fluorescence emitters within a protective host shell, segregating them from the reactive photocrosslinking moieties on the surface. The site-specific isolation ensures that crosslinking reactions occur at the periphery, leaving the emissive cores intact and preserving high electroluminescence. We demonstrate robust processing orthogonality in sequential multilayer ELPR photolithography, enabling sub-diffraction fluorescence nanopatterns with critical dimensions down to 110 nm. Remarkably, deactivation of G-ortho-P-Br to G-ortho-P-deBr leads to an 18-fold increase in maximum external quantum efficiencies (EQEs, from 1.6% to 30.3%) and a 17-fold enhancement in current efficiency (from 4.25 to 75.44 cd A^{-1}). Finally, we validate the EL performance of various ELPRs with full-color, UV-patterned OLEDs exhibiting EQEs exceeding 13% [1]. These results not only pave the way for extending Moore's Law to organic optoelectronics but also unlock their potential for monolithic optoelectronic integration.

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References

[1] S.-W. Lo, S. B Shivarudraiah, Z.-H. Lin, P. Helbling, L. Song, J. Wang, M. Nouman, F. Jiang, J. Zhu, M.-N. Chen, S. Kumar, H. Wang, A. J Christofferson, Y. Bao, and C.-J. Shih, Chemrxiv, https://doi.org/10.26434/chemrxiv.10001854/v2 (2026).

Electron Boost: Novel n-Dopants for Organic Photovoltaics

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Doping is a crucial concept in semiconductor technology, and it is no different for organic semiconductors. It increases conductivity and facilitates carrier injection and extraction. While substantial success has been achieved for organic molecular p-dopants, the same cannot be said for n-dopants. They suffer from an inherent disadvantage: the highest occupied molecular orbital (HOMO) of the n-dopant must lie below the lowest unoccupied molecular orbital (LUMO) of the host, rendering them typically unstable under ambient conditions. Here, we report a new and efficient molecular n-dopant that can dope C60 to a conductivity of 24 S/cm. It can also achieve a low activation energy of 25 meV, the lowest reported for n-doped organic thin films [1]. We investigate the origin of its efficacy and explore the doping mechanism. Moreover, we incorporate the new n-dopant into organic solar cells, demonstrating its effectiveness by improving the power conversion efficiency of the reference devices.

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References
Schwarze et al., Nature Mater, 18, 242–248 (2019)

Electropolymerized Polyaniline Copolymers on Carbon Fibers for Supercapacitor Applications

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Carbon fiber electrodes coated with conductive polymers have emerged as promising materials for advanced energy storage devices due to their high pseudocapacitance, good electrical conductivity, and mechanical flexibility. Recent studies have shown that conductive polymer composites combined with carbon substrates can significantly enhance the electrochemical performance of supercapacitor electrodes [1,2]. In this work, conductive polymer films were electropolymerized directly onto carbon fiber (CF) electrodes using aniline in combination with 3,4-ethylenedioxythiophene (EDOT) and p-phenylenediamine (PPD), forming polyaniline-based copolymeric systems. This strategy aims to combine the high conductivity of PEDOT, the pseudocapacitive properties of polyaniline, and the redox activity of PPD to improve charge storage and ion transport within the electrode structure. The electrochemical performance of the electrodes was investigated using cyclic voltammetry (CV), galvanostatic charge–discharge (GCD), and electrochemical impedance spectroscopy (EIS). The copolymeric electrodes exhibited higher redox activity and larger voltammetric areas compared with individual polymers and the pristine carbon fiber electrode. Among the investigated systems, the PANI–PPD3 electrode showed the best performance, reaching a maximum areal capacitance of 835 F cm^{-2} at 1 A cm^{-2}, together with good rate capability. Impedance analysis revealed reduced charge-transfer resistance and improved ionic transport. These results demonstrate that electropolymerized conductive polymer copolymers on carbon fibers are promising electrode materials for high-performance supercapacitors.

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References
[1] Rangel, AMS, Babu, RS, Vinayagam, M., Samyn, LM, Vinodh, R., & de Barros, ALF. Materials Letters , v. 398, p. 138897 (2025)

[2] Samyn, LM, Babu, RS, Devendiran, M., & De Barros, ALF. Ionics , v. 26, n. 6, p. 3041-3050

Fabrication and temperature-dependent magnetotransport of organic spin valves using an NDI-based semiconductor active layer

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Organic spin-valve devices are promising for spintronic applications because of their long spin coherence[1–2], but their magnetotransport is also sensitive to interfacial structure and film morphology. Here, we fabricate vertical spin valves based on the NDI-based semiconductor T2-(NDI-T2)$_2$-2EH, with films spin-coated on NiFe and a transferred Co top electrode. Clear MR signals are observed only in as-cast devices at low temperatures. The mismatch between MR peaks and coercive fields indicates additional interfacial contributions, including spin-dependent trapping, local magnetic interactions, and field-history-dependent scattering.

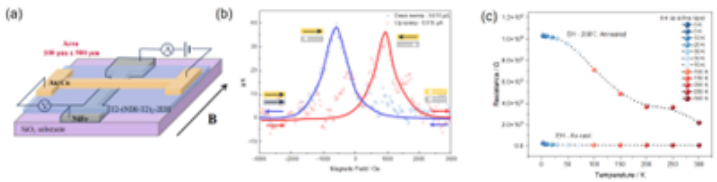


Figure 1. (a) Device schematic. (b) MR–H curves at 3 K. (c) Resistance vs. temperature.

After annealing, the MR signal disappears, and the device resistance increases by about one order of magnitude. Although crystallinity has improved, device performance has declined because the rougher surface morphology increases interfacial resistance and leads to uneven contact. Overall, these results show that magnetotransport in vertical organic spin valves is dominated by interface structure and contact quality. Improved crystallinity alone does not guarantee better performance, highlighting the importance of interface engineering in organic spintronic devices.

Acknowledgements
Funded by the DFG – TRR 386 – TP B5,number 514664767.

References

J. Devkota, R. Geng, R. C. Subedi, et al., Advanced Functional Materials, 26, 3881 (2016)

Y. Zheng, Y. Feng, D. Gao, et al., Advanced Electronic Materials, 5, 1900318 (2019)

From Growth Conditions to Thermal Response: Reversible Polymorphism in SiPc Thin Films

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In this work, we report a thermally controlled and reversible polymorphic transition in silicon phthalocyanines (SiPc), manifested as a rapid structural rearrangement upon heating with a slow recovery when cooled down. While similar temperature-driven responses accompanied by pronounced mechanical effects have been observed in other classes of organic semiconductors[1], this is, to our knowledge, the first observation of such behavior in an SiPc system. We suspect that this response originates from the incorporation of siloxane substituents into the molecular structure, similar to other bulky chains structures that have presented this kind of behaviour[2]. The transition was investigated using a combination of in situ X-ray diffraction, in situ atomic force microscopy, and in situ Raman spectroscopy, allowing direct correlation between structural, morphological, and molecular-level changes during thermal cycling. In situ XRD reveals a complete and reversible phase transformation occurring below 70 °C, a relativelly low transition temperature compare to other materials in literature[2]. Furthermore, by modifying the surface chemistry during deposition, we observe clear changes in the transition kinetics, demonstrating that fabrication parameters influence not only the initial crystalline structure but also its thermal evolution. When integrated into organic thin-film transistors, this polymorphic transition leads to pronounced and reversible changes in electrical properties, more than one order of magnitud in mobility values, directly linking structural dynamics to device performance. These results establish thermally controlled polymorphism as a functional stimulus-response mechanism in siloxane-SiPc systems and highlight a promising design space for smart electronic materials, including thermally responsive devices, memories, and thermally activated actuators[5].

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References

S. Kyu Park, Y. Diao, Chem. Soc. Rev. 2020, 49, 8287.

D. W. Davies, B. Seo, S. K. Park, S. B. Shiring, H. Chung, P. Kafle, D. Yuan, J. W. Strzalka, R. Weber, X. Zhu, B. M. Savoie, Y. Diao, Nat. Commun. 2023, 14, 1304.

S. K. Park, H. Sun, H. Chung, B. B. Patel, F. Zhang, D. W. Davies, T. J. Woods, K. Zhao, Y.

Diao, Angew. Chem. Int. Ed. 2020, 59, 13004.

Furan-Based A-D-A Non-Fullerene Acceptors for Organic Photovoltaics

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With the rapid growth in the performance of organic photovoltaic (OPV) technology, it becomes essential to incorporate intrinsic stability and sustainability into material design in preparation for their future commercialization. Currently, most non-fullerene acceptors (NFAs) rely on petroleum-derived thiophene and its derivatives as building blocks, while alternatives, such as furan — a more biodegradable and better pi-conjugated analog — remain largely unexplored due to discouraging initial results. Recently, our group demonstrated that using furan can increase both the efficiency and the photostability of the NFA.1,2 In this presentation, we will discuss the advantages and limitations of replacing thiophene units in NFAs with their furan counterparts. We will show how this structural modification affects the compounds' electronic properties, solid-state packing, and photovoltaic properties. We will discuss the photodegradation pathways of NFA compounds (photocyclization vs photoxidation), and how the placement of furan in various positions of NFA, including ring-fused systems3 influences the materials photovoltaic efficiency and photostability.

References

Che, Y.; et al. Design of Furan-Based Acceptors for Organic Photovoltaics. Angew. Chem. Int. Ed. 2023, 62 (40), e202309003

Che, Y.; et al. Mechanism of the Photodegradation of A-D-A Acceptors for Organic Photovoltaics. Angew. Chem. Int. Ed. 2021, 60 (47), 24833-24837

Wei, M. et al. Benzofuran-Based Non-Fullerene Acceptor with Low Voltage Loss for Organic Photovoltaics, in preparation

High-performance hybrid supercapacitors based on magnesium molybdenum selenide architecture and biomass carbon

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Recently, the demand for energy storage devices is rapidly increasing to meet the requirements for broad applications in the 4th industrial revolution era. Among various energy storage devices, hybrid supercapacitors have great attention owing to high power/energy densities, fast charge/discharge cycling, good durability, environmental friendliness, and low cost [1]. Particularly, binary metal selenide-based electrode materials are very promising because of their high chemical stability and better redox activity [2]. In this presentation, we report magnesium molybdenum selenide electrode materials synthesized by a facile hydrothermal method, together with selenium incorporation for supercapacitor applications [3]. The fabricated materials showed a nanosphere morphology composed of polyhedral-like structures. The influence of Se incorporation on the nanostructure and electrochemical performance was investigated. Also, biomass-derived porous activated carbon was developed for negative electrode, which provides ultra-long cycling stability. A hybrid supercapacitor was fabricated, indicating high specific capacitance performance and long-term cycling stability. These results suggest that the magnesium molybdenum selenide and biomass carbon materials have a great potential as supercapacitor electrodes for next-generation advanced energy storage applications.

References

S. Zhang, W. Zhao, S. He, T. Li, and J. Luo, J. Power Sources, 666, 239209 (2026).

V. K. Mariappan, M. H. P. Puthanveettil, M. Singh, S. C. Amarakonda, and S. Dasgupta, J. Energy Storage, 145, 119898 (2026).

M. Nagaraju, G. S. R. Raju, S. Swathi, K. Pravallika, and J. S. Yu, (2026), Submitted.

High-performance Y6 homojunction organic solar cells

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Non-fullerene small molecule acceptor (NFA) materials have enabled bulk heterojunction (BHJ) organic photovoltaic (OPV) devices to exceed 20% power conversion efficiency (PCE). However, BHJ film morphology can be challenging to reproduce and scale up for commercial manufacturing. Single material active layer (i.e., homojunction) architectures could significantly simplify the large-scale fabrication process, but solution-processed homojunction OPV devices have so far achieved only modest PCEs < 1.5%. Recent studies of the optoelectronic properties of the NFA Y6 have described its capability to achieve spontaneous free charge generation, making it a strong candidate for improving homojunction device performance. I will present the results from a systematic investigation into how device architecture and the choice of charge transport layers affect Y6 homojunction OPV performance. We find the choice of the charge transport layers to be critical to ensuring efficient charge extraction from the Y6 layer, with maximum PCEs exceeding 2.5% – the highest reported efficiency for any solution-processed small molecule homojunction OPV device to date.[1] The improved efficiency was attributed to the inclusion of a TFB layer and its electron blocking and hole extraction properties. The PCE was further improved up to 5.4% through control of the Y6 active layer nanostructure via the use of additives.[2] These findings establish homojunction active layers as a promising route to efficient and scalable OSCs and highlight the prospect for further performance gains through the tuning of active layer nanostructure and the device architecture.

References

Shaun McAnally et al., Small 21, 2409485 (2025)

Shaun McAnally et al., Advanced Energy Materials 16, e04807 (2026)

Highly Conductive Porous MOF Thin Films Enabled by Controlled Interfacial Oxidation

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Liquid–liquid interfacial polymerisation can yield highly ordered conductive metal–organic frameworks, but for porous nitrogen-based systems such as $Ni_3(HITP)_2$ it has been difficult both to access a true interfacial growth route and to control the ligand oxidation needed for extended π–d conjugation[1]. Here we introduce controlled interfacial oxidation, in which molecular oxygen is metered from an immiscible organic phase during liquid–liquid interfacial polymerisation. This establishes a robust interfacial synthesis platform and decouples two orthogonal controls: precursor stoichiometry, which determines structural order, and dissolved O_2 concentration, which controls ligand oxidation and electronic connectivity. Applied to $Ni_3(HITP)_2$, this strategy yields highly ordered porous thin films with room-temperature electrical conductivity up to 626.5 S/cm and near-metallic transport, with only ~5% increase in conductivity between 110 and 270 K. As the dissolved O_2 concentration is reduced during synthesis, the conductivity drops and its temperature dependence strengthens monotonically, showing that controlled ligand oxidation drives the system toward the metallic side of the crossover once high structural quality is achieved. The optimised films also deliver a thermoelectric power factor of 18.1 μW m^{-1} K^{-2}, an order-of-magnitude improvement over previous $Ni_3(HITP)_2$ reports and among the highest values reported for a porous MOF[2]. Controlled interfacial oxidation therefore provides a synthetic route to combining exceptional crystallinity, very high electrical conductivity, and strong thermoelectric performance with intrinsic porosity in conductive frameworks.

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References

[1] Dennis Sheberla et. al. J. Am. Chem. Soc. 2014, 136, 25, 8859–8862

[2] Lei Sun et. al. Joule 2017, 1, 1, 168-177

Hybrids of Conducting Polymers and Graphene Derivatives for Electrochemical Sensor Applications

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In the development of hybrids based on conducting polymers (CPs) and carbon materials such as graphene derivatives (GDs), the choice of parameters such as composition, synthesis methodology, and deposition technique is key to achieving the desired properties. In our research group, we have prepared different hybrids based on CPs such as polyaniline (PAni), polypyrrole (PPy), and poly(ortho-ethoxyaniline) (POEA), combined with GDs such as graphene oxide and its reduced form (GO and rGO, respectively).

Handmade screen-printed electrodes were fabricated on polyester substrates using a conductive ink based on an alkyd resin and graphite. These hybrids were produced via two different routes: chemical synthesis and electropolymerization. The chemically synthesized hybrids were incorporated into the conductive inks, while the electropolymerized hybrids were deposited directly onto the working electrode surface.

The mass ratio between the monomers and GDs was varied from 1 to 10% (w/w). The electrodes were characterized by Fourier-transform infrared spectroscopy (FTIR), Raman spectroscopy, scanning electron microscopy (SEM), and electrochemical techniques such as cyclic voltammetry (CV) and electrochemical impedance spectroscopy (EIS).

The results showed that both the mass ratio and the method used to obtain the hybrids play a fundamental role in their electrochemical properties. It was observed that a low mass ratio of GDs in the hybrids can significantly decrease the charge transfer resistance (Rct) while preserving the redox characteristics of the original CPs. In addition, some of these hybrids were evaluated in sensor applications, such as the determination of progesterone and as taste sensors. The hybrid-based electrodes exhibited increased sensitivity and selectivity [1–5].

Acknowledgements
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References
De Araújo GM, Cardoso MA, Codognoto L, et al (2023) Screen-Printed Electrodes Based on Conductive Inks of Polyaniline/Graphene Hybrids and Their Application to Progesterone Detection. ECS Adv 2:016504. https://doi.org/10.1149/2754-2734/acbeca

De Araújo GM, Cardoso MA, Carnaúba JHS, et al (2025) Electrochemical study of screen-printed electrodes modified with electropolymerized polyaniline films grafted with low mass ratio of graphene oxide. J Solid State Electrochem 29:1093–1103. https://doi.org/10.1007/s10008-024-05981-9

Carnaúba JHS, De Araújo GM, Cardoso MA, et al (2024) Screen-printed electrodes based on hybrids of poly(ortho-ethoxyaniline) and reduced graphene oxide. Diam Relat Mater 144:111029. https://doi.org/10.1016/j.diamond.2024.111029

Improved performance of PM6:Y6-based organic solar cells by introducing a layer of metallic nanoparticles into its structure.

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The efficiency of bulk heterojunction organic solar cells (BHJOSCs) has surpassed the 20% barrier. However, the high recombination of photocarriers, especially at the interfaces of their layers, poses significant obstacles to be overcome. The present work aims to introduce nanoparticles between different layers of BHJOSCs, in an interface engineering process, aiming to reduce recombination losses [1]. First, we compared two solar cells using PM6:Y6 as active layers and PEDOT:PSS as the HTL: one in which silver nanoparticles (AgNPs) were incorporated in between the HTL and active layer, and other without nanoparticles. Second, a similar BHJOSC structure, having Br-2PACz as HTL, with and without the introduction os Au ou MoO3 nanoparticles between the transparent electrode and the HTL layer. Electrical analyses were conducted using steady-state current-voltage (J-V), Photo-CELIV, and current and voltage transients (TPC and TPV) measurements. The analysis was complemented by fitting the experimental results by an analytical expression for the photocurrent that assumes second-order kinetics for bimolecular recombination [2]. The introduction of nanoparticles produced a significant improvement in the parameters of organic solar cells, increasing the efficiency of some cells by almost 2%.

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References

D. Brenes-Badilha, D. J. Coutinho, D. R. B. Amorim, R. M. Faria, and M. C. Salvadori, Journal of Applied Physics, v. 123, n. 15, p. 155502, 2018.

D. R. B. Amorim, D. J. Coutinho, P. B. Miranda, and R. M. Faria, Physical Review Applied, v. 14, p. 034046, 2020.

Improving charge extraction in organic photoanodes via n-type SAM modification of buried ZnO/organic interfaces

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Organic photoanodes for photoelectrochemical (PEC) water splitting can be limited by charge-extraction losses and interfacial recombination within multilayer stacks, particularly at buried contacts. Here, we modify the buried interface between a ZnO electron transport layer and an organic photoactive layer by inserting an n-type self-assembled monolayer (SAM) as a molecular interlayer. The interlayer is formed from an n-type conjugated material bearing a phosphonic-acid anchoring group, which binds to the ZnO surface and adjusts the local chemical and electronic environment. This buried-interface modification reduces defect-related loss channels and yields more favorable interfacial energetics, enabling more efficient electron extraction and suppressed recombination. In particular, the molecular interlayer is expected to passivate interfacial trap sites and to mitigate energetic barriers at the ZnO/organic contact, thereby improving charge selectivity at the buried interface. Consequently, devices show lower dark current, improved photovoltage characteristics, and higher photocurrent, consistent with reduced parasitic leakage pathways and more effective carrier collection under illumination. We fabricate organic photoanodes by integrating a NiFe layered double hydroxide (NiFe-LDH) oxygen-evolution catalyst and evaluate PEC performance in alkaline electrolyte[1]. Compared to the reference without SAM, the SAM-modified photoanode exhibits a cathodically shifted onset potential from 0.61 to 0.56 V vs. RHE and a higher photocurrent density at 1.23 V vs. RHE from 23.58 to 24.81 mA cm–2, resulting in an outstanding half–solar-to-hydrogen conversion efficiency of 7.89%. Overall, these results highlight n-type SAM-based buried-interface tuning as a practical strategy to improve charge extraction and reliability in organic PEC photoelectrodes.

References

Yu, J. M., Lee, J., Kim, Y. S., Cho, S., Yang, C., Jang, J. W., Nature communications, 11(1), 5509. (2020)

Interface Regulation of Oxygen Evolution Cocatalysts towards Efficient Solar-Driven Water Splitting

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Developing efficient and low-cost oxygen evolution cocatalysts (OECs) is an effective approach to address the sluggish surface catalytic reactions of photoanodes. Currently, common OECs loading strategies involve hydrothermal treatment or spin coating directly onto the photoanode surface, introducing new interfaces within the photoelectronic devices: the interface between the photoanode and OECs (P/C interface). The simple overlay of OECs on the photoanode inevitably results in numerous defects at the P/C interface, leading to severe recombination of photogenerated carriers and hindering device performance. Therefore, a high-quality P/C interface (with few defects, strong bonding, and facilitation of photogenerated carrier transfer) is crucial for the efficient transfer of photogenerated electron-hole pairs and is key to OECs design. This study employs in-situ loading of OECs and low-temperature thermal treatment to fabricate composite photoanode devices with high-quality P/C interfaces on metal sulfide-based photoanodes, thereby enhancing the overall photoelectrochemical performance of the devices.

References

L. Meng, J. He, X. Zhou, K. Deng, W. Xu, P. Kidkhunthod, R. Long, Y. Tang, L. Li, Nat. Commun. 12, 5247 (2021)

L. Meng, X. Zhou, S. Wang, Y. Zhou , W. Tian, P. Kidkhunthod, S. Tunmee, Y. Tang, R. Long, Y. Xin, L. Li, Angew. Chem. Int. Ed. 58, 16668, (2019)

L. Meng, Z. Lv, W. Xu, W. Tian, L. Li, Adv. Sci. 10, 2206729, (2023)

Interfacial Siloxane Interactions to Enhance Semiconductor Ordering and Performance in Organic Thin-Film Transistors.

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Achieving low-power, high-mobility organic thin-film transistors (OTFTs) requires control over the buried interface between the semiconductor and dielectric layers. Here, we demonstrate that siloxane-based molecular design provides a powerful means to engineer interfacial compatibility and charge transport. By integrating siloxane-functionalized diketopyrrolopyrrole (DPP) semiconductors with a PDMS based polyionic liquid dielectric, we show that siloxane–siloxane interactions promote enhanced molecular ordering, increased crystal coherence, and improved charge-carrier mobility of the semiconductor. Grazing-incidence wide-angle X-ray scattering and Raman morphological analyses indicate that interfacial interactions drive coherent stacking and reduce disorder at the interface. This interfacial design strategy offers a general approach to tuning interfaces through conjugated polymer/dielectric systems, offering insight into strategies for the development of low-voltage, high-performance organic electronics.

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The work was conducted through contributions of all authors. L.E.D. conducted the experimental work and data analysis. H.C. synthesized PDMS-PSS and determined conditions to enable for capacitor films to be fabricated. V.D. assisted in the characterization of the dielectric material. N.K., S.M. and N.Lec designed and synthesized the DPP-Si polymer. N.L. assisted in the GIWAXS analysis. K.U.M. and C.-H.K. performed the device simulation and modeling. J.G.M. (CG Figures) provided the graphics used in the figures, as well as assisted in AFM imaging and processing. B.H.L. acquired funding, managed supervision, directed the study, and assisted in editing the manuscript. The authors would also like to thank Dr. Halynne Lamontagne and Bahar Ronnasi for their assistance in data analysis. They would also like to extend their thanks to the SOLEIL Synchrotron and Dr. Arnaud Hemmerle for their assistance and time during beamline use. We thank Natural Sciences and Engineering Research Council of Canada (NSERC) Discovery program (#162583 to B.H.L.) for supporting this project. We thank the Canadian Foundation for Innovation, CFI# 40178 (HIIT) and CFI# 43247 (SSMART), for support in acquisition and maintenance of the infrastructure needed for this project. This work was also supported by NSERC Discovery Grant RGPIN-2024-04589 (C.-H.K.) and NSERC PGS-D (L.E.D.).

References

Dickson, L. E.; Cho, H.; Ledos, N.; Dipalo, V., Mohanan, K. U.; Manion, J. G.; Kamatham, N.; Méry, S.; Leclerc, N.; Chang-Hyun Kim.; Lessard, B. H. Mater. Horiz (2025). Under Review.

Investigating Structure-Property Relationships of Poly(Ionic Liquids) for Gating Materials in Organic Thin-Film Transistors

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Enabling low-cost fabrication of flexible electronics is highly dependent on the development of easily processable and high-performing polymeric materials for organic thin-film transistors (OTFT). Although there have been significant efforts to optimize the semiconducting materials of OTFTs, dielectric gating materials remain much less explored, while having a significant impact on device performance. Poly(ionic liquids) (PILs) are attractive dielectric materials for low-power organic thin-film transistors due to their high capacitance, printing compatibility, and recyclability capabilities. PILs retain many of the unique physicochemical characteristics of ionic liquids while overcoming several of their practical limitations by remaining in the solid state. In addition, the molecular structure and composition of the PIL play a crucial role in the dielectric performance. Polymer architecture, monomer selection, molecular weight, functional groups, and counter ions all contribute to the behaviour of the final PIL and ultimately the OTFT performance. The molecular tunability distinguishes PILs from many conventional dielectric materials, which typically offer only limited avenues for chemical modification. This research investigates how polymer structure influences capacitance, ionic conductivity, polarization rates, and overall dielectric performance when integrated into OTFTs. Identifying these structure-property relationships helps optimize the balance between high capacitance and insulating properties when developing PILs for OTFT applications. PILs consisting of styrenics, vinyl pyridines, viologens and tertiary amine methacrylates are synthesized and characterized with structural modifications made to polymer architecture, alkyl chain length and

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The work was conducted through contributions of all authors. V.D. Synthezied all PIL materials, conducted the experimental work and data analysis. H.C assisted in determining monomer and polymerization parameters as well as material characterization. L.E.D assisted in OTFT device fabrication and data analysis. S.M. assisted in the integration and characterization of the PILs in capacitors. B.H.L. acquired funding, managed supervision and directed the study, and assisted in editing the manuscript. We thank Natural Sciences and Engineering Research Council of Canada (NSERC) Discovery program (#162583 to B.H.L.) for supporting this project. We thank the Canadian Foundation for Innovation, CFI# 40178 (HIIT) and CFI# 43247 (SSMART), for support in acquisition and maintenance of the infrastructure needed for this project. This work was also supported by NSERC PGS-D (L.E.D.).

References

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Kinetic Monte Carlo modelling of organic optoelectronic devices for optical communication

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Organic light emitting diodes (OLEDs) and photodiodes (OPDs) present compelling alternatives to their inorganic counterparts in optical communication owing to their spectral tunability and the absence of toxic or resource critical elements. A possible downside could be the low charge-carrier mobility of organic semiconductors, but when high biases are applied one can profit from the strong field enhancement of the mobility. Current modelling of organic optoelectronic devices predominantly relies on rate equation or drift-diffusion approaches, which are insufficient in describing the coupled charge transport and excitonic processes occurring at the molecular up to the device scale. Mechanistic Kinetic Monte Carlo (kMC) simulations can capture all these processes at all relevant spatial and time scales, and are therefore perfectly suitable to explore the fundamental mechanisms that ultimately constrain data rates and device performance. In this work, we employ kMC simulations to analyse the reported transient behaviour of an OLED [1] and an OPD [2] driven by a sequences of voltage or optical pulses, respectively. By systematically varying the repetition rates and key device/material parameters, we study their impact on the luminescence and photocurrent transients, as well as on the spatiotemporal evolution of excitons and charges inside the devices. We find that the bandwidth in both devices can be greatly reduced by increasing the bias voltage, demonstrating the feasibility of using OLEDs and OPDs in optical communication with speeds that can compete with their inorganic analogues.

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References

K. Yoshida et al., Nature 621, 746 (2023).

S. Ullbrich et al., J. Phys.Chem. Lett. 8(22), 5621 (2017).

Large scale determination of frontier orbital energies in small molecule organic semiconductors via exciplexes

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Important parameters in modelling organic electronic devices in are the energies of the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO). These energy values are often found electrochemically or spectroscopically, and often need corrections or have a large uncertainty. Herein we present a simple, yet unique method of determining such energy levels using photoluminescence spectra of 1:1 donor:acceptor blends that show intermolecular charge-transfer states (exciplexes). The optical peak energy from such exciplexes will then be defined as the difference between the donor HOMO and the acceptor LUMO minus an effective exciplex binding energy. Assuming that this exciplex binding energy is constant, a graph of measured exciplex optical energies can be made using many commonly used donor and acceptor molecules. It is possible to then determine the HOMO/LUMO for all such donor-acceptor pairs by solving a linear system of equations. This method has been applied using more than 550 spectra, 160 donors and 180 acceptors. It is easily scalable and thus far is accurate to better than 0.1 eV. We use as a calibration material the fluorescent organic semiconductor □-MADN, which has been well studied [1,2] and allows for the determination of accurate absolute values for the HOMO and LUMOs. A key finding is that the ‘effective exciplex binding energy’ used in solving the linear system shows a surprisingly small variation, better than 0.1 eV, within the database [3]. The method is validated using a comparison with spectroscopic data. The effective binding energy, which is close to 1.0 eV, is argued to be given by the sum of the adiabatic exciplex binding energy and shifts due to energetic relaxation, exciplex-vibron coupling and a Stokes shift. We expect this database to continue growing by the addition of exciplex data for new donor and acceptor materials. It thus provides an accurate and growing basis for predictive device simulations

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References

G. Tirimbo et al. Phys. Rev. B 112, 224203 (2025)

E.J. de Jong et al., Phys. Rev. B 112, 224204 (2025)

C. B. McDonald et al. (Advanced Materials, under review)

Mapping Electric-Fields within Polymeric Field-Effect Transistors by Sum-Frequency Microscopy

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Organic Field-Effect Transistors (OFETs) are the basis of organic electronics, just as inorganic transistors are fundamental building blocks to current (inorganic-based) electronics. Among their main advantages are low cost, simple fabrication, and versatility, made possible by the chemical design of the organic semiconductor properties. Although the basic working principle of an OFET is well understood [1], testing current OFET models against experimental data is scarce in the literature [2], especially regarding the charge density distribution within the channel of operating OFETs. In this study, all-polymer OFETs based on the semiconductor P3HT and the polar dielectric PMMA were fabricated and characterized, yielding electrical parameters consistent with those reported in the literature. Sum-Frequency Generation (SFG) vibrational spectroscopy is used for probing the electric field in the PMMA dielectric layer during device operation [3]. Using an SFG microscope recently developed in our laboratory, we have imaged the generated SFG signal within the OFET channel throughout its operation, both in the linear and saturation regimes. The images revealed a non-uniform field (accumulated charge) distribution along the channel, with average intensity patterns partially consistent with theoretical models, including the gradual channel approximation and the model proposed by Schmechel et al. [2], which suggests charge inversion at a specific point within the channel (pinch off). Such charge inversion is indeed evidenced for the first time by a change in the SFG lineshape of the C=O vibration. These studies will allow unprecedented comparisons of experimental and theoretical charge distribution profiles in OFETs, which may significantly improve our understanding of their operation principles.

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References

G. Horowitz, J. Mater. Res. 19, 1946-1962 (2004)

R. Schmechel, M. Ahles, H. von Seggern, J. Appl. Phys. 98, 084511 (2005)

S.G. Motti, L. S. Cardoso, D. J. C. Gomes, R. M. Faria, P. B. Miranda, J. Phys. Chem. C 122, 10450-10458 (2018)

Materials Acceleration Platforms: toward the laboratory of the future for perovskite and organic PV research

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The development of complex functional materials poses a multi-objective optimization problem in a large multi-dimensional parameter space. Solving it requires reproducible, user-independent laboratory work and intelligent preselection of experiments. However, experimental materials science is a field where manual routines are still predominant, although other domains like medicine, biotechnology or pharmacy have long used robotics and automation. As the number of publications on Materials Acceleration Platforms (MAPs) increases steadily, we review selected systems [1,2] and fit them into the stages of a general material development process to examine the evolution of MAPs up to the AMANDA (Autonomous Materials and Device Application) platform [3]. Subsequently, we present our newest approach to lab automation for perovksite and organic PV research with the example of precise time-controlled quenching processes for perovskite film formation with solvent, gas and vacuum and autonomous perovskite film deposition optimization using automated optical characterization (Abs, photoluminescence) and machine learning for planning of the next generation of experiments.

References

Y. Zhao, et al., Nature communications 12(1), 2191

S. Langner, et al., Journal of Materials Science 56, 16422-16446, (2021)

J. Wagner, et al., Advanced Materials 32 (14), 1907801, (2021)

Microstructural Studies of Solution-Processed Organic Optoelectronic Materials

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Solution-processed organic semiconductors, including organic solar cells and photodetectors, have witnessed remarkable progress in recent years due to their compatibility with large-area, flexible fabrication. Beyond the development of novel materials and device engineering, optimizing device performance through precise control of thin-film morphology remains a critical challenge. The complexity of bulk-heterojunction (BHJ) architectures and the rapid dynamics during film formation hinder effective morphology control during processing. In this talk, we integrate molecular dynamics simulations with *in situ* and *ex situ* nanoscale structural characterizations to systematically investigate the morphological evolution during film deposition. Our results reveal that the molecular conformation of donor and acceptor materials in solution, along with specific interactions between the acceptor and the solvent, govern the sensitivity of the final morphology to solvent choice. By leveraging this understanding, we successfully realized solvent-insensitive organic solar cells. Furthermore, we extended this morphological control strategy to circularly polarized organic photodetectors, demonstrating promising potential for near-infrared CPL detection applications.

Acknowledgements
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References

Solvent insensitive high efficiencies of organic solar cells reveal the key factors for morphology control. Nature Energy, 2025, 10, 1, 124-134.

Sensitive near-infrared circularly polarized light detection via non-fullerene acceptor blends. Nature Photonics, 2023, 17, 649-655.

A guest-assisted molecular-organization approach for >17% efficiency organic solar cells using environmentally friendly solvents. Nature Energy, 2021, 6, 1045-1053.

Modeling steady-state responses of organic electrochemical transistors based on drift-diffusion fundamentals

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Organic Electrochemical Transistors (OECTs) have emerged as key components in bioelectronics, sensors, and neuromorphic computing due to their high transconductance, low operating voltage, and compatibility with solution processing. [1] Despite their widespread application, a comprehensive theoretical framework describing the interplay between ionic and electronic transport in organic mixed ionic-electronic conductors (OMIECs) remains an open challenge. Most existing models, including the widely used Bernards-Malliaras (BM) capacitive model, [2] successfully describe OECT behavior but fall short in explaining how extracted device parameters relate to material composition. In this work, we introduce a drift-diffusion approach to determine ion uptake in the mixed conductor. We derive an analytical expression for the steady-state current in p-type, depletion-mode OECTs based on PEDOT:PSS. Our model explicitly incorporates material properties such as the salt concentration in the electrolyte and intrinsic hole-charrier concentrations the OMIEC. To evaluate our model, we compare it to experimental I-V characteristics. Furthermore, we extend the BM model and a thermodynamic approach, [3] establishing interconversion relations between their parameters. This comparative analysis reveals that different theoretical frameworks, despite their distinct physical foundations, can yield similar experimental fits, emphasizing the need for careful parameter interpretation.

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Funding by FAPESP (2018/15670-5, 2023/15105-4) CNPq (304662/2025-9) and CAPES (finance code 001) is acknowledged.

References

[1] R. Colucci et al., Flex. Print. Electron. 5 (2020), 013001

[2] D.A. Bernards et al. Adv. Funct. Mat. 17 (2007), 3538

[3] M. Cucchi, et al. Nat. Comm. 13 (2022), 4514

Molecular Weight Engineering of PSS for Enhanced Thermoelectric Properties in PEDOT:PSS

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Global electricity consumption is increasing at an average annual rate of approximately 2.4%, while nearly 76% of this demand is still supplied by fossil fuels, intensifying greenhouse gas emissions. Simultaneously, roughly 60% of the world's energy is dissipated as waste heat from industrial processes, engines, and electronic devices. The direct conversion of this waste heat into electricity through thermoelectric devices represents a strategic approach to mitigate energy losses and reduce environmental impact.(1) Although inorganic materials exhibit high thermoelectric performance, their toxicity, rigidity, and high production costs limit large-scale applications. In this context, conducting polymers emerge as promising alternatives due to their intrinsic mechanical flexibility, low cost, solution processability, and scalability. Among them, poly(3,4-ethylenedioxythiophene):poly(styrene sulfonate) (PEDOT:PSS) stands out as one of the most versatile systems, combining chemical stability, aqueous processability, and tunable electrical properties.(2) Despite recent advances, the relationship between the molecular weight of the poly(styrene sulfonate) (PSS) and the thermoelectric performance of PEDOT:PSS remains insufficiently understood. In this work, we demonstrate that engineering the molecular weight of PSS is a key parameter for optimizing charge transport and power factor. Increasing the molecular weight promotes the formation of larger, interconnected PEDOT-rich domains, enabling more efficient conductive pathways. The formulation based on PSS of 157 kDa achieved a power factor of (1.33 ± 0.03) μW/(K2·m), approximately 30 times higher than that obtained for the system containing PSS of 23 kDa. These findings demonstrate that molecular control of PSS represents a decisive strategy to enhance the thermoelectric performance of PEDOT:PSS-based inks, opening new ways for high-efficiency polymeric materials for waste heat recovery.

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References
DiSalvo FJ. Thermoelectric Cooling and Power Generation. Science (1979). 1999 Jul 30;285(5428):703–6. doi:10.1126/science.285.5428.703

Culebras M, Gómez C, Cantarero A. Review on Polymers for Thermoelectric Applications. Materials. 2014 Sep 18;7(9):6701–32. doi:10.3390/ma7096701

Multiscale Interface Engineering in Conjugated Polymers and Hybrid Perovskites

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Interfacial processes critically influence charge transport, ionic migration, defect formation and degradation pathways in emerging optoelectronic materials, making their control essential for improving the performance and stability of photovoltaic systems based on conjugated polymers and hybrid perovskites. In electrochemically deposited PAni/P3HT bilayers, spectroscopic analyses indicate energy transfer from photoexcited PAni chains to P3HT domains, while structural characterization reveals polaron formation and irregular aggregate growth affecting interchain transport. In $MAPbI_3$ thin films, modulation of the antisolvent volume during spin coating controls crystallization dynamics, altering grain size distribution and grain-boundary density and providing direct evidence for the intrinsic origin of current–voltage hysteresis. Substrate effects in multication FA-Cs films show that samples deposited on FTO exhibit enhanced resistance to thermal and humidity-induced degradation compared to PEDOT:PSS, with structural analyses revealing phase segregation and halide redistribution. Defect-mediated recombination was mitigated through incorporation of the chelating molecule salophen during $MAPbI_3$ processing, whose coordination with Pb^{2+} improves crystallization, reduces residual PbI_2 and promotes hydrophobic surface formation, leading to enhanced charge extraction and efficiencies above 18% under ambient conditions. Additionally, electrochemically synthesized H_3PO_4-doped polyaniline was implemented as a hole transport layer, enabling efficiencies of 11.5% and improved fill factor, demonstrating that interface engineering across molecular and microstructural scales provides an effective strategy to reduce hysteresis, enhance stability and optimize charge-carrier dynamics in next-generation photovoltaic devices.

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References

G. A. S. Felício et al, Phys. Scr. 101, 045509 (2026)

A. Morais et al, J. Mater. Chem. A, 3, 33175 (2025)

Narrowband absorbing aggregates of merocyanine dyes in solution and solid state

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The specific molecular arrangement and the number of π-stacked organic molecules within a molecular aggregate strongly influence the resulting optical properties. Dipolar merocyanine dyes typically assemble in an antiparallel, H-type fashion, whereas the formation of more intriguing J-type structures has only rarely been reported.[1] Here, we demonstrate for a series of mono- and bis-merocyanines featuring the same π-scaffold — and thus identical monomeric properties — that the aggregate structure can be precisely controlled through variation of the chromophore substituents and the spacer moiety. This structural control enables strong excitonic coupling within either card-stack (H-type) or zig-zag (J-type) arrangements, both of which exhibit exchange narrowing into a single, high-intensity excitonic band. Further tuning of the optical properties is achieved through subtle chemical modifications of isostructural chromophores as well as by blending them into hybrid materials.[2] This enables us to control the aggregate size in solution and different matrix materials, up to extended assemblies in the crystalline solid-state. The resulting tunable narrowband absorption can be exploited in organic photodiodes for wavelength-selective photocurrent generation, achieving external quantum efficiencies of up to 11% and ultranarrow bandwidths of 11 nm.[2,3] Overall, linewidth narrowing in optoelectronic functional materials via excitonic coupling represents a powerful strategy for the development of ultra-narrowband absorbers suitable for sensing applications.

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References

[1] J.-H. Kim, T. Schembri, D. Bialas, M. Stolte and F. Würthner, Adv. Mater. 34, 2104678, (2022)

[2] T. Schembri, J. Albert, H. Hebling, V. Stepanenko, O. Anhalt, K. Shoyama, M. Stolte and F. Würthner, ACS Central Sci. 11, 452 (2025)

[3] A. Liess, A. Arjona-Esteban, A. Kudzus, J. Albert, A.-M. Krause, A. Lv, M. Stolte, K. Meerholz, F. Würthner, Adv. Funct. Mater. 29, 1805058 (2019)

Organic complementary inverters based on inverted coplanar thin-film transistors employing different contact functionalization

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Since organic semiconductors can be processed at or near room temperature, they provide the possibility to fabricate displays and sensors on flexible polymeric substrates. For such mobile systems, a low power consumption is a prerequisite. Since the complementary circuit design results in significantly smaller static power consumption compared to the unipolar circuit design, it is favored. Organic complementary circuits are typically based on p-channel and n-channel thin-film transistors (TFTs) fabricated using two different organic semiconductors. If the TFTs are fabricated in the inverted coplanar device architecture, the source/drain contacts are often functionalized with a chemisorbed molecular monolayer to minimize the contact resistance. For p-channel TFTs, pentafluorobenzenethiol (PFBT) has emerged as the most promising thiol for this purpose, while for n-channel TFTs, 4-(methylsulfanyl)-thiophenol (MeSTP) has shown excellent results. The challenge is to functionalize the contacts of p- and the n-channel TFTs on the same substrate with different thiols. Here, we demonstrate a fabrication scheme that allows the functionalization of the p-channel TFTs with PFBT and of the n-channel TFTs with MeSTP. The success of this fabrication scheme is supported by photoelectron spectroscopy (XPS) and time-of-flight secondary ion mass spectrometry (ToF-SIMS). We compare the measured static and dynamic performance of two types of flexible organic complementary inverters, one in which the contacts of the p- and n-channel TFTs were functionalized using the same thiol (PFBT), and one in which the contacts of the n-channel TFTs were functionalized using MeSTP and those of the p-channel TFTs with PFBT. For the latter, the inverters have small-signal gains as large as 100, noise margins as large as 70% of half-the-supply voltage, and characteristic signal-delay time constants of less than 2 µs at a supply voltage of 2 V.

References

T. Leydecker, et al., Chem. Soc. Rev., 49, 7627, (2020)

J. W. Borchert, et al., Adv. Mater., 34, 2104075, (2022)

S. Steffens, et al., ACS Appl. Mater. Interfaces, 18, 2162, (2026)

Persistent radicals in for pattern recognition of electrical and multicolor optical stimuli

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Organic photonic synaptic transistors (OPSTs) integrate light detection and signal processing, memory, and computation capabilities due to their intrinsic multifunctionality. Multiple and uncorrelated strategies have been used to achieve memory characteristics by photo-inducing trapping sites in the different functional layers of OPSTs. However, none of them are grounded in a purely molecular engineering and chemical design approach of constituent materials.

Here, an innovative solution-processed OPST that works as a multiple-stimuli synaptic device is proposed by implementing a persistent organic radical capable of multiple wavelength photoexcitation in the photoactive layer and a ferroelectric polymer as the dielectric layer that exhibits electrically induced polarization. Persistent organic radicals exhibit a unique electronic structure characterized by a singly occupied molecular orbital, endowing them with inherent multifunctionality for light emission, light sensing, and information storage [1, 2].

Theoretical calculations demonstrated that long-term memory is enabled by the photogeneration of specific trap states in the radical component of the photoactive layer of the OPST, thus clearly correlating the molecular electronic configuration and neuromorphic properties in such prototypal organic compounds. We exploit the intrinsic multifunctionality of the radical-based OPST (i.e. providing both electrical and multicolor optical stimulations) for emulating dendrite integration which is a neuromorphic feature rarely explored but fundamental to perform spatiotemporal pattern discrimination and network-level computation (i.e. for artificial retina applications) [3].

Finally, the further configuration of the OPST is endowed with a light-emission functionality thus providing synaptic-like facilitation/depression in electroluminescence intensity once the device is subjected to pulsed illumination and/or subsequent electrical inputs.

References

G. Baroni et al., ACS Applied Electronic Materials, 7, 3694–3703 (2025).

F. Reginato et al., Advanced Functional Materials, 35, 2411845 (2025).

G. Baroni et al., Materials Horizons, DOI: 10.1039/d5mh01710f

Processing-structure-property relationship in fully solution processed multilayer P(VDF-TrFE) piezoelectrics

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Fully solution processed polymer piezoelectrics enable scalable electromechanical devices compatible with flexible substrates and large area manufacturing. This talk presents advances in multilayer P(VDF-TrFE) piezoelectric architectures fabricated entirely by solution deposition, including printed electrodes, dielectric interfaces, and ferroelectric layers. Layer by layer processing reveals how confinement, interfacial fields, and sequential crystallization influence effective d33, charge generation, and dielectric loss relative to single layer films. We show that polymer solubility in solution differ from the kinetics governing dissolution of the semicrystalline solid during over coating. Leveraging this distinction, we identify solvents with slow film dissolution that prevent redissolution and stabilize the multilayer fabrication. Although each solvent exhibits distinct drying temperature dependent yield behavior, their maximum yields and piezoelectric responses converge. This decoupling isolates the roles of drying temperature, which sets defect formation and breakdown pathways, and annealing temperature, which drives ferroelectric phase development and remnant polarization. A systematic study of poling parameters enables a practical method for identifying optimal poling conditions. Using these insights, we fabricate multilayer devices with up to five active layers, achieving charge densities up to 376 μC/m², surpassing state of the art triboelectric nanogenerators. I conclude with implications for scalable, cost effective roll to roll manufacturing and demonstrations of multilayer devices charging capacitors and driving small electronics.

References

Abhishake Goyal, Dongze Wang, Yanguang Zhang, John Weber, Gaozhi Xiao, Jianping Lu, Chun-il Kim, Jun Gao, Salima Alem, Journal of Polymer Science 63, 2903-2912 (2025).

Shiyu Hu, Yanguang Zhang, Dongze Wang, John Weber, Shoude Chang, Gaozhi Xiao,Jianping Lu, Neil Graddage, Jun Gao, Tahmid Rakin Siddiqui, Suprabha Islam,Chun-il Kim, Ye Tao, Advanced Materials Technologies 10, 2401009 (2025).

Skew-Gaussian Device Design and Application for Realistic Gaussian Distribution Representation

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As artificial intelligence increasingly operates in noisy and uncertain real-world environments, hardware platforms capable of directly processing statistical information are highly desirable [1-3]. Here, we present a skew-Gaussian-like device based on a twist contact architecture that intrinsically emulates asymmetric Gaussian distributions at the device level. By selectively configuring the top or bottom contact as the source electrode, contact-dependent carrier injection and extraction asymmetry induces either right- or left-skewed Gaussian-like current responses without additional control voltages. This approach enables energy- and area-efficient realization of diverse Gaussian distributions within a single device. To demonstrate practical applicability, the proposed device was integrated into a hardware system for credit card transaction analysis, achieving a fraud-detection accuracy of 95.8%. These results highlight the potential of twist-contact-based skew-Gaussian devices as a scalable and efficient building block for hardware-integrated probabilistic and uncertainty-aware computing.

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References

Sebastian, A., et al. Nature communications, 10(1), 4199.

Cho, J., et al. Advanced Materials, e11018.

Beck, M. E., et al. Nature communications, 11(1), 1565.

Surfactant-free organic nanoparticle dispersions for light-harvesting applications

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Solution deposition from nanoparticle dispersions allows the use of eco-friendly processing agents such as alcohols or water for the fabrication of organic semiconductor thin-films for optoelectronic applications. Primary application of the eco-friendly device production from organic nanoparticles are solar cells where solvents are evaporated on large scale upon drying. Omitting surfactants to stabilize the dispersions is essential to not jeopardize the device performance. In this work, novel surfactant-free nanoparticle dispersions from high-performance organic semiconductors are synthesized by nanoprecipitation and electrostatically stabilized by electrical doping. The corresponding solar cells achieved power conversion efficiencies beyond 10%, matching the performance of reference solar cells deposited from toxic solvents. When applied to organic photodetectors, the nanoparticle approach allows the fabrication of thick absorber layers which enhance the quantum efficiency in the outer parts of the absorption spectrum, yielding enhanced broad-band detectivity. Aqueous dispersions of the organic semiconductor nanoparticles can be used for catalytic hydrogen generation.

References

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Temperature-dependent structural fluctuations govern charge transport in hybrid tin-halide perovskites thin film transistors

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Hybrid halide perovskites are attracting growing interest as high-mobility, solution-processable semiconductors for thin-film transistors (TFTs). In this context, tin-based halide perovskites are particularly attractive as they offer reduced ionic screening compared to lead-based analogues and reported mobilities μ > 50 cm2 V-1 s-1. [1] Despite remarkable TFT performance, a detailed understanding of long-range charge transport in perovskite semiconductors is still limited and often complicated by dynamic disorder, charge trapping, ionic screening and contact-limited effects.[2] Here, we discuss the impact of temperature-dependent structural dynamics on charge transport in the archetypal polycrystalline Cs0.1FA0.9SnI3. By extracting reliable transport parameters from temperature-dependent four-point-probe transfer curves and gated Hall measurements, we measure room-temperature hole mobilities up to 12 cm2 V-1 s-1 and identify thermally activated transport with temperature-dependent activation energy. We further observe a pronounced increase in mobility with increasing field-induced hole density. By correlating transport with temperature-dependent GIWAXS, vibrational spectroscopy, photoluminescence and large-scale molecular-dynamics simulations, we show that mobility and photoluminescence brightness track the evolution of dynamic disorder linked to soft-lattice structural fluctuations. [3] Furthermore, we propose a multiple-trapping-and-release model that rationalises the temperature dependence of charge-carrier mobility through changes in the trap density of states and highlights the impact of impurity scattering as mobility-limiting mechanism in polycrystalline perovskite films. This comprehensive picture of charge transport in tin-halide perovskites provides design guidelines for high-mobility perovskite transistors and informs the understanding of transport processes relevant to other optoelectronic devices, including solar cells and LEDs.

Acknowledgements
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References

Liu, A., Zhu, H., Bai, S. et al., High-performance metal halide perovskite transistors. Nat Electron 6, 559–571 (2023)

Y. Zhang, S. Pecorario, X. W. Chua, et al., Critical Assessment of Contact Resistance and Mobility in Tin Perovskite Field-Effect Transistors. Adv. Electron. Mater. 11, no. 15 (2025): e00924.

S. Pecorario, P. Ahlawat, Y. Zhang., X. Chen, R. Mazlumian, M. Dubajic, I. Jacobs, H. Sirringhaus et al., Temperature-dependent structural fluctuations govern charge transport in hybrid tin-halide perovskites thin film transistors. To be submitted, 2026

Template Quality Dependent Conversion Synthesis of Boron Nitride Coated Graphene Hybrid Aerogels for Ultrasensitive and Selective Ammonia Sensing

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Hexagonal boron nitride (h-BN) is generally considered unsuitable for gas adsorption, though theoretical studies suggest that introducing charge or defects can make h-BN effective for this purpose. Previous studies have used carbon materials as templates for synthesizing h-BN, but the effect of template quality on the reaction has not been explored. BN aerogels (BNAs) were synthesized using graphene aerogels (GAs) of different qualities as the template, using ammonia gas as the nitrogen source and boric acid powder as the boron source. In the thermal reduction reaction, boron and nitrogen elements replace the carbon elements in graphene. Depending on the quality of the graphene template and the reaction conditions, pure BNA or BN/graphene hybrid aerogels (BNGAs) are formed. BNGA can be further annealed in air at 700 oC to remove the graphene template and obtain pure BNA. BNGAs can be integrated into the chemical-sensitive FET chip for localized deposition of the sensing layer. We have discovered for the first time in this system that the difficulty of conversion in the template synthesis of h-BN is positively correlated with the quality of the carbon template, an observation that is verified on both graphene nanosheets and carbon nanotubes. h-BN and graphene coexist in BNGA and exhibit a 3D folded morphology similar to GA, maintaining the porous structure. BNGA is used for ammonia gas sensing, with a detection limit as low as 20 ppb and high selectivity. Through density functional theory calculations, the adsorption energy and charge transfer between NH3 molecules and BNGA are greatly enhanced. This innovative approach promises new possibilities for the application of h-BN in gas sensing, with the potential to play a significant role in gas capture, environmental monitoring, and other related fields.

References

H. Long, Adv. Funct. Mater. 26, 5158, (2016)

Terminal group effects on SAMs packing and perovskite interfacial energetics

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Self-assembled monolayers (SAMs) have emerged as highly efficient hole-selective contacts for inverted perovskite solar cells. [1-3] However, a fundamental understanding of how molecular structure governs monolayer packing and perovskite interfacial energetics remains limited, particularly under air-ambient processing conditions. Here, we report the design and synthesis of two novel triphenylamine-based phosphonic acid SAMs featuring electron-withdrawing (F) and electron-donating (OMe) terminal groups, alongside a neutral analogue, to systematically investigate terminal group effects on interfacial properties. The triphenylamine (TPA) core was selected as a rigid and synthetically accessible scaffold that combines well-established hole-transporting characteristics with broad modularity, enabling straightforward structural functionalization through conventional coupling. Using AFM-IR nanoscale chemical mapping, we demonstrate that terminal group electronics directly dictate SAM packing density and homogeneity, with methoxy substitution yielding the densest and most uniform monolayers. Ultraviolet photoelectron spectroscopy reveals that this enhanced packing is accompanied by favorable interfacial dipole formation and improved energetic alignment with the valence band of $FAPbI_3$. These interfacial modifications impact perovskite film growth via a two-step deposition process under ambient conditions, leading to compact, void-free films and enhanced interfacial hole extraction, as confirmed by steady-state and time-resolved photoluminescence measurements. In contrast, electron-withdrawing terminal groups result in sparse monolayer coverage, unfavorable energetic offsets, and inefficient charge transfer. This work identifies terminal group engineering within rigid TPA-based SAMs as a key strategy to control molecular packing, interfacial energetics, and perovskite growth, providing molecular-level design guidelines for robust, air-processed perovskite photovoltaics.

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authors acknowledge the Atomic Force Microscopy, and Ultraviolet Photoelectron Spectroscopy staff for their assistance during the experiments (proposal nos. 20242995 and 20252101).

References

Yang, Jie; et.al. Nature Communications, 16, 6968, 2025.

Jiang, Wenlin; et.al. Nature, 646, 95–101, 2025.

Wu, Wenping; et.al. Science, 389, 195-199, 2025.

Thermal potential induced redox reaction enabled ionic thermoelectric generator

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The ionic thermoelectric (iTE) effect is well known in the field of thermal energy harvesting. It is based on the thermodiffusion of ions with different mobility along a temperature gradient between the electrodes, generating a thermal potential. Ionic thermoelectric devices generate thermal potentials typically two orders of magnitude higher than classic electronic-based thermoelectric generators (higher Seebeck coefficients), but are unable to generate continuous power output, due to the inability of ions to pass through electrodes. Thermogalvanic cells (TGCs), another thermal energy harvesting device, are based on the entropy difference between a reversible redox couple upon temperature difference between the electrodes. They can provide constant power extraction when connecting a load to the electrodes, due to the electron transfer between the redox molecules and the electrode. In this work, we proposed a new mechanism to generate constant power from an iTE cell, where continuous current output is enabled by the thermal voltage induced redox reaction, while keeping high Seebeck coefficient from ionic thermodiffusion. In this new type of device, called ionic thermoelectric generator (iTEG), self-assembled polyethylene glycol (PEG) clusters stabilized by alkoxide end groups in a PEG/NaOH water electrolyte was identified to be the key composition for the redox reaction. The optimized device delivered 100 mV at 20 K of temperature difference and maximum power density of 4.2 mW m-2. These discoveries establish a new design principle for iTE devices and pave the way towards the development of energy devices and technologies, such as batteries, sensors and other electrochemical ion/electron coupled devices.

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References
Candiotto de Oliveira, P. et al. Thermal potential induced redox reaction enabled ionic thermoelectric generator. Nano Energy. 148, 2026.

Thermoelectric Properties of Thiophene-Based N-type Copolymers in Doped Oriented Thin Films

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While thermoelectric devices are currently made from inorganic materials,1 a great deal of attention is being paid to highly conductive organic polymers that can be processed in solution and easily integrated into flexible, portable devices. While p-doped organic polymers have demonstrated high power factors and high electrical conductivities approaching,2 n-doped counterparts still lag behind, primarily due to limited charge-carrier mobility and suboptimal doping efficiency. Achieving high electrical conductivity in n-type polymers remains a challenge, often hindered by inefficient doping and inappropriate chemical alternated D-A chemical structures. In this work, we report the development of high-performance n-type polymers for organic thermoelectric applications. The materials were processed via a solution-based approach that integrates high-temperature rubbing (HTR) to promote polymer chain orientation with sequential doping, using the n-type dopant N-DMBI-H, to enhance dopant incorporation. Molecular design strategies, specifically the introduction of weak non-covalent interactions and fused-ring backbones, were employed to improve backbone planarization and charge transport. As a result, the optimized materials achieved a power factor exceeding 100 $\mu W \cdot m^{-1} \cdot K^{-2}$, demonstrating the effectiveness of combining structural design and process engineering.

References

1. Hasan, Md. N.; Wahid, H.; Nayan, N.; Mohamed Ali, M. S. Inorganic Thermoelectric Materials: A Review. Int. J. Energy Res. 2020, 44 (8), 6170–6222. https://doi.org/10.1002/er.5313.

2. Durand, P.; Zeng, H.; Biskup, T.; Vijayakumar, V.; Untilova, V.; Kiefer, C.; Heinrich, B.; Herrmann, L.; Brinkmann, M.; Leclerc, N. Single Ether-Based Side Chains in Conjugated Polymers: Toward Power Factors of 2.9 mW M−1 K−2. Adv. Energy Mater. 2022, 12 (2), 2103049. https://doi.org/10.1002/aenm.202103049.

Thermogalvanic Cells Towards Large-scale Applications

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Thermogalvanic cells (TGCs) are highly promising for recovering low-grade waste heat (below 100 °C) due to their low-cost materials, scalable fabrication, and relatively high Seebeck coefficients (1–2 mV K^{-1}). TGCs operate by imposing a temperature gradient across two electrodes immersed in an electrolyte containing redox-active species. The resulting thermovoltage arises from the entropy difference between oxidized and reduced species (Se = $\Delta S_r c/nF$), enabling continuous power generation under stable thermal gradients. Despite their potential, realizing TGCs for large-scale applications remains challenging, particularly in the modular integration of multiple cells into thermogalvanic modules (TGMs) with sufficient voltage and power outputs. Here, we present a fully printed TGM prototype consisting of 36 serially connected cells. The module employs screen-printed hybrid current collectors, activated carbon electrodes, a laser-drilled spacer, and a pressure-sensitive adhesive layer to ensure robust assembly and thermal sealing. Using aqueous electrolytes, the TGM delivers a reproducible thermopower of 38 mV K^{-1} and a peak output power of 9 µW under a 14 K temperature gradient. We have also explored the improving effect of polyelectrolyte on the thermal power and output performance of TGCs. This work demonstrates a scalable platform for low-cost, flexible thermoelectric harvesting and lays the groundwork for practical deployment of TGMs in waste heat recovery systems. It also offers a versatile design concept applicable to other electrolyte-based energy conversion devices.

Acknowledgements
EU commission under the project Metatherm, Swedish Research Council (Project 2024-04196)

References
1. Pedro Santos Candiotto de Oliveira, Ujwala Ail, Zia Ullah Khan, Reverant Crispin, Dan Zhao. Adv. Energy Sustainability Res. 2025, 2400428

Tin perovskite quasi-2D thin films transistors: devices and low temperature charge transport study

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Metal halide tin perovskite films emerged in the last few decades as an environmentally friendly alternative to their lead-based counterpart for the realization of optoelectronic devices like solar cells. However, their properties make them ideal candidates also for p-type thin film transistors, expanding the plethora of possible applications and providing a powerful platform for the study of their transport properties [1].

In this work we present p-type, tin perovskite thin film transistors characterized by a quasi-2D composition obtained by optimizing the ratio between formamidinium and a spacer cation (phenethylammonium), which resulted in devices showing field-independent linear mobilities up to 7 $cm^2v^{-1}s^{-1}$, on/off ratio of 10^6, and threshold voltages lower than 10 V. While a few works have already studied the low temperature behavior of similar structures, they are limited by the use of liquid nitrogen to a minimum of around 80 K [2,3]. Here, charge transport properties were studied by liquid Helium, low temperature measurements down to 10 K. The increase of current and mobility with increasing temperature previously reported is confirmed in a similar range, while a different trend is observed at the lowest temperatures, characterized by a significant shift in the subthreshold swing and in general in the diffusion-dominated part of the trans characteristic curves. Such trends are then discussed in terms of the characteristic properties of metal halide perovskites while keeping in consideration also the geometrical constraints imposed by the device structures.

This study therefore highlights the transport properties of these materials, providing insights into their working principles and future strategies for optimizing both electronic and optoelectronic devices based on metal halide perovskites.

Acknowledgements
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References

[1] Liu, A., Zhu, H., Bai, S. et al. High-performance metal halide perovskite transistors. Nat Electron 6, 559–571 (2023). https://doi-org.proxy-ub.rug.nl/10.1038/s41928-023-01001-2

[2] Y.Zhang, S.Pecorario, X. W.Chua, et al. “Critical Assessment of Contact Resistance and Mobility in Tin Perovskite Field-Effect Transistors.” Adv. Electron. Mater.11, no. 15 (2025): e00924. https://doi.org/10.1002/aelm.202400924

[3] B.Jeong, L.Veith, T. J. A. M.Smolders, M. J.Wolf, K.Asadi, Room-Temperature Halide Perovskite Field-Effect Transistors by Ion Transport Mitigation. Adv. Mater.2021, 33, 2100486. https://doi.org/10.1002/adma.202100486

Triplet loss processes in phosphorescent OLEDs: an integrated study

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Modern OLEDs make use of phosphorescent emitter molecules containing heavy atoms like Pt or Ir, where the spin-orbit coupling (SOC) enables radiative decay of triplet excitons. However, the SOC also enables long-range Förster-type transfer of the triplet excitons to excited molecules carrying an electron or hole polaron, or another triplet exciton. This gives rise to triplet-polaron quenching (TPQ) and triplet-triplet annihilation (TTA), respectively, and therefore triplet loss. The rate of such Förster-type transfer is proportional to the spectral overlap between the emission spectrum of the phosphorescent emitter and the absorption spectrum of the acceptor molecule carrying a polaron or triplet exciton. We report on an integrated study of TPQ and TTA that involves photophysical experiments, spectroelectrochemical experiments measuring the absorption spectrum of charged molecules [1], kinetic Monte Carlo simulations of polaron and exciton dynamics and interactions, and quantum-chemical calculations of ground state and excited-state properties of several phosphorescent emitter and host materials. We find that in some host-emitter systems, like m-MTDATA:Ir(ppy)2acac, a correct quantification of TPQ between a triplet exciton on an emitter molecule and a polaron on the host molecule requires going beyond Förster theory, which includes only dipole-dipole coupling, by including also dipole-quadrupole coupling between the triplet exciton and the polaron [2]. In the case of TTA between two triplet excitons on emitter molecules, we find that the TTA rate generally decreases with increasing emission energy, in agreement with experimental results. However, emitter-specific exceptionally large or small TTA rates occur because of coincidentally large or small overlaps between the emission and absorption spectra [3]. Our results will be helpful in finding material systems where triplet loss processes and associated material degradation are minimized.

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References

[1] S.E.A. Jaspars, H. Tomita, C. van Hoesel, N. Daub, R.A.J. Janssen, and R. Coehoorn, Adv. Funct. Mater. 35, 2425548 (2025).

[2] C. van Hoesel, R. Coehoorn, and P.A. Bobbert, Phys. Rev. B 111, 224204 (2025).

[3] C. van Hoesel, C.S. Chibueze, L. Visscher, R. Coehoorn, and P.A. Bobbert, to be published.

Tunable stability and performance of fused thienothiophene based polymers for organic electrochemical transistors and artificial synapse based on a side chain reorganization strategy

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We report a series of novel polythiophene-based polymeric mixed ionic-electronic conductors, based upon the incorporation of fused thieno[3,2-*b*]thiophene and bithiophene with isomeric sidechains. The enhanced rigidity in the polymer backbone facilitated the formation of stabilized bipolarons, while the reorganized ethylene glycol side chains not only maintained the polymer's hydrophilicity but also unexpectedly enhanced the crystallinity of polymer film. This design strategy led to the development of 4gTT-2gT, a high-performance and stable organic mixed ionic-electronic conductor. The polymer exhibited a maximum μC^* of 729 F V^{-1} cm^{-1} s^{-1}, one of the highest values among low-threshold voltage polythiophene derivatives, while demonstrating excellent operational stability, retaining 99% of its maximum current after one-hour device switching cycles and 94% after nine-hours at lower bias. We implemented the material in OECT-based artificial synapses, which maintained functionality under a large temperature range (233 K to 373 K). These combined properties establish 4gTT-2gT as a prime candidate for next-generation mixed conductor devices.

References

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Understanding the impact of structural defects in conjugated polymers across various device types

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Alternating conjugated polymers, central to the performance of organic electronics, are often idealized as perfectly ordered structures. In reality, structural defects, particularly homocoupling defects introduced during cross-coupling polymerizations like Stille, are commonly present and can significantly affect material properties and device performance. These imperfections disrupt backbone regularity, reduce molecular weight, increase dispersity, and contribute to poor batch-to-batch reproducibility, thus limiting commercial scalability. While previous studies have demonstrated that homocoupling defects can adversely affect the performance of organic electronics, including organic photovoltaics (OPVs), photodetectors (OPDs), and organic electrochemical transistors (OECTs), a comprehensive understanding of their impact across these diverse device platforms remains incomplete. Here, we address this knowledge gap through a comparative study of traditionally synthesized alkoxy- and glycolated PBTTT/pgBTTT polymers and their newly developed homocoupling-free analogues. Using scanning tunneling microscopy (STM), we directly quantify and spatially map homocoupling defects in these materials, revealing distributions that are not fully captured by conventional characterization techniques such as MALDI-ToF mass spectrometry. We also study the impact of defects on mechanical properties, crucial in obtaining flexible devices. We further demonstrate significant OECT improvement using defect-free materials which underscores the need for structurally well-defined systems in understanding mixed ionic-electronic transport. By integrating structural, electronic, and device-level analyses across multiple application contexts, this study demonstrates the critical influence of molecular defects and makes a compelling case for the development and deployment of homocoupling-free semiconducting polymers in next-generation organic electronics.

References

J. Vanderspikken, Z. Liu, et al., Adv. Funct. Mater., 33, 2309403 (2023).

Z. Liu, J. Vanderspikken, et al., Adv. Funct. Mater, 2413647 (2024).

L. Bynens, P. Mantegazza et al., J. Am. Chem. Soc., jacs.5c19024 (2026).

Understanding the underlying processes behind high performing organic homojunction solar cells

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In the last decade, organic solar cells (OSCs) have seen significant increases in their power conversion efficiencies (PCEs), which are nearing 20% due to the development of novel non-fullerene acceptors (NFAs). An interesting feature of some NFAs, such as Y6, is that they appear to have moderate yields of free charge carrier generation upon photoexcitation, which has led them to be explored as active layer materials for homojunction OSCs. Homojunction OSCs are potentially simpler to reproducibly fabricate at scale than bulk heterojunctions and have seen increasing interest. Despite the absence of a donor material, homojunction OSCs with PCEs surpassing 5% have been recently reported [1]. These devices both raise many fundamental questions and offer an opportunity to gain insights into the charge generation and recombination processes of high-performing non-fullerene materials. In this work, I will describe how the pairing of drift-diffusion modelling with experimental measurements can be employed to investigate the performance characteristics of homojunction OSCs. I will discuss the factors that drive the relatively high short-circuit current and the observed inverse relationship between device PCE and open-circuit voltage. I will describe the role played by charge-transfer (CT) states that form at the interface of Y6 subdomains, and how several trends can only be explained by invoking these states. I will discuss the impact of solvent additives on active layer morphology, and how morphology impacts CT state energy, charge generation, and bimolecular recombination. These insights are of broader relevance to understanding the performance of BHJs, wherein the underlying mechanisms by which the NFA contributes towards charge generation, and recombination are not fully understood.

References

S. McAnally, E. Brooks, H. Jin, et al. “Y6 Homojunction Organic Solar Cells with Over 5% Power Conversion Efficiency by Controlling the Active Layer Morphology.” Advanced Energy Materials 16, no. 5 (2026): e04807. https://doi.org/10.1002/aenm.202504807

Unraveling electronic structure from 2D to 2D/3D perovskite interfaces by UV-vis, electron and photoelectron spectroscopy

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Two-dimensional (2D) halide perovskites are important for improving the efficiency and stability of perovskite optoelectronics. While their crystal structure and band-gap widening are widely discussed, the understanding of energy level position and how it relates to the choice of spacer cation remains limited. To shed light on this, we systematically investigated how the alkylammonium spacer lengths (C3–C10) affect the crystal structure, band gap, and electronic structure of 2D Ruddlesden–Popper perovskites (A'_2PbI_4, n = 1) using XRD, UV–vis, UPS, and DFT. Interestingly, no correlation between spacer length and band gap was found, rather a pronounced odd–even effect, with odd-numbered spacers showing up to 90 meV larger band gaps. DFT links this behavior to variation in packing, leading to a spacer-length-dependent Pb–I–Pb bond-angle distortions. Furthermore, we found that despite the pronounced band-gap widening, the ionization energy remains nearly constant across the series and only slightly larger than that of 3D $MAPbI_3$, indicating that the band gap increase mainly results from an upward shift of the conduction band minimum. Beyond pure 2D systems, we also investigated low-dimensional surface phases formed by depositing bulky ammonium spacer (PEA, phenethylammonium) onto 3D films. Angle-resolved X-ray photoelectron spectroscopy (AR-XPS) allows us to distinguish signals originating from the 3D layer and the low-dimensional capping layer. These measurements reveal gradual compositional gradients rather than abrupt interfaces. Notably, annealing and post-washing can significantly reshape near-surface cation distributions. To establish a correlation between interfacial composition and band-gap evolution, we employ reflection electron energy loss spectroscopy (REELS) at varying excitation energies. Using these complementary techniques allows us to draw a comprehensive picture of the near-surface electronic structure and band-gap evolution at 2D/3D interfaces.

References

J. Mater. Chem. A, 2025,13, 18935-18947

Unveiling degradation differences of perovskite PV: from cells to modules.

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Perovskite Solar Cells (PSCs) have emerged as one of the most promising next-generation photovoltaic technologies due to their rapid efficiency improvements, reaching the record of 26.95% at the laboratory scale. [1] Despite this remarkable progress, device stability remains a major barrier to commercialization. While most stability studies focus on small-area laboratory cells, practical deployment requires large-area modules where additional degradation pathways may arise. This work discusses the differences in degradation mechanisms observed when scaling PSCs from individual cells to modules. Cells and modules were fabricated via solution process techniques (blade and slot-die coating) under ambient conditions and over flexible substrates. Through the analysis of different characterization techniques (I-V, EQE, UV-Vis, PL, EL, XRD), we analyze key intrinsic degradation pathways occurring under damp heat, thermal and light exposure and how module-level factors—including laser scribing, electrical interconnections and mechanical stress—introduce new failure modes. Among the differences detected, it was shown that cells under light stress suffer mostly from a loss in current, while modules show decrease in fill factor and sudden failures due to the interconnections. The tests also reveal reproducibility issues, which are directly linked to the lack of uniformity in the deposition of PSC using solution-based methods – a significant challenge for the technology scale-up.

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References
[1] NRL, Best Research-Cell Efficiency Chart, retrieved from https://www.nlr.gov/pv/cell-efficiency on 03-16-2026.

UVA sensor based on conducting polymer

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Monitoring of ultraviolet is important for health, industrial and environmental applications. Commercial inorganic UV photodetectors have high selectivity and stability, but their intrinsic hardness and high-temperature processing methods are unsatisfactory. Organic photodetectors enable solution processing and intrinsic flexibility, but are typically limited by their complex device structures and limited integration density. In this study, we demonstrate an air-operable UVA sensor based on a single conducting polymer. UVA illumination fills oxygen-related traps, increases carrier density and enables a two-terminal device with a wide light intensity range (0.2~500 mW/cm2), large current change rate (~60%), well-defined intensity-time-dependent responses, and reversible reset through defect reconfiguration. We achieve flexible sensors, high density integration arrays (576/cm2) and optoelectronic information encryption for applications. We further present organic photoelectrochemical transistors that couple light signals with electrochemical gating to achieve synapse-like functions. This strategy offers broad application prospects and a versatile design framework for next-generation organic optoelectronic systems.

References

Xing, S., Bittrich, E., Prifti, V. et al. Light-induced fine-tuning of optical cavities for organic optoelectronic devices. Nat Commun 16, 8426 (2025). https://doi.org/10.1038/s41467-025-64272-7

Wavelength-Selective Negative Photoconductance in ZnON phototransistor for Neuromorphic Vision

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Negative photoconductance (NPC) was demonstrated in zinc oxynitride (ZnON) phototransistor enabled by a ZnON/ZnO heterojunction formed through nitrogen volatilization during annealing. The built-in potential at the heterointerface allowed highly sensitive photoresponse at operating voltages below 1 V and under ultralow light intensities of several μW/cm^2. The devices exhibited wavelength-dependent NPC behavior, suppressing leakage current under ambient illumination, with red light inducing synaptic potentiation and green and blue light causing synaptic depression. Furthermore, the wavelength-dependent response enabled discrimination of the correlated color temperature of white light and image color correction mimicking human visual perception, highlighting ZnON phototransistor as multifunctional platforms for energy-efficient sensing and memory-integrated optoelectronic systems.

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References
He, W., Wu, D., Kong, L., Yu, P., & Yang, G. (2024). Giant negative photoresponse in van der Waals graphene/AgBiP2Se6/graphene trilayer heterostructures. Advanced Materials, 36(16), 2312541.

ZnO thin films deposited by PE-PLD for gas sensing applications

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Zinc oxide (ZnO) is a wide-bandgap semiconductor known for its high optical transparency, electron mobility, and chemical stability, making it a promising material for electronic and sensing applications [1]. In this work, ZnO thin films were deposited by plasma-enhanced pulsed laser deposition (PE-PLD) using a dual radiofrequency (RF) plasma source. The incorporation of a background RF plasma enhances the ionization of ablated species, while the dual RF configuration enables independent control of ion energy and ion flux through the low-frequency (LF) and high-frequency (HF) components, respectively [2]. This study investigates the influence of deposition parameters, including substrate temperature and RF power, on the structural, optical, and surface properties of ZnO thin films. The films were characterized by optical profilometry, X-ray diffraction (XRD), atomic force microscopy (AFM), and UV-Vis spectroscopy to evaluate their physical and optical properties. Preliminary results show a strong correlation between deposition conditions and film properties such as surface morphology and optical transmittance. Further characterization by X-ray photoelectron spectroscopy (XPS), field-emission scanning electron microscopy (FESEM), and Raman spectroscopy is currently underway to gain deeper insight into the surface chemistry, microstructure, and defect-related properties of the films. In parallel, gas sensing measurements are being conducted to evaluate the performance of the films in sensing applications. These results highlight the potential of PE-PLD-grown ZnO thin films for gas sensing and their relevance for integration into electronic sensing platforms.

Acknowledgements
This work is funded by FONDECYT 1220359.

References

Jacques Perriere, et al., Pulsed Laser Deposition of Thin Films: Application Led Growth of functional Materials, John Wiley & Sons (2007), págs. 261-289.

Boyle, P. C., et al., Journal of Physics D: Applied Physics, 37(5), 697-701.

π–d Conjugated Coordination Polymers for Thermoelectric and Solar Energy Applications

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Coordination polymers based on dithiolene ligands are emerging as intrinsically conductive materials for sustainable energy applications, combining π–d conjugation, redox activity and structural tunability without the need for dopants.1,2 However, their intrinsic insolubility has historically limited processability and device integration.3 Here we report the synthesis and additive-free processing of Ni- and Cu-based coordination polymers, poly[Kx(Niett)] (Niett) and poly[Kx(Cuett)] (Cuett), as thermoelectric and electrocatalytic materials. Stable dispersions were obtained in polar solvents due to electrostatic stabilization of the counterion, enabling homogeneous thin-film deposition at room temperature. Both materials exhibit narrow bandgaps (<1.0 eV), decomposition temperatures above 200 °C and electrical conductivities up to 10^{0} S cm^{-1} in thin-film configuration. Periodic DFT calculations rationalize the metal-dependent electronic structure and reproduce the opposite Seebeck behaviour of the two systems. Planar and flexible p–n thermoelectric modules assembled from Cuett and Niett display Seebeck coefficients (200 μV K^{-1}) and output power approaching the algebraic sum of the single legs. Beyond thermoelectrics, the synthesized coordination polymers have also been investigated as counter electrodes in dye-sensitized solar cells. Niett thin films exhibit low charge-transfer resistance (8.0 Ω cm^{2}), high exchange current density (5.5 mA cm^{-2}), and full devices delivered photoconversion efficiencies above 10%, exceeding state-of-the-art PEDOT control. This work establishes additive-free processed dithiolene coordination polymers as intrinsically conductive, multifunctional platforms for thin-film electronic devices, bridging coordination chemistry and synthetic electronic materials for sustainable energy technologies.

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References

G. H. Morritt, H. Michaels and M. Freitag, Chemical Physics Reviews 3, 011306 (2022)

R. Eisenberg and H. B. Gray, Inorganic Chemistry 50, 9741 (2011)

N. Fan, W. You, W. Gong, F. Jiao and W. Hu, Materials Today Chemistry 47, 102808 (2025)

A Dilute-Heterojunction Strategy for Probing Charge Generation in Organic Photovoltaics

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Recent advances in non-fullerene acceptors (NFAs) have enabled organic photovoltaics (OPVs) to surpass 20% power-conversion efficiency. Despite this progress, the microscopic mechanisms governing efficient charge generation remain incompletely understood, largely due to the complex and highly intermixed morphology of bulk heterojunction (BHJ) blends. Such structural heterogeneity makes it difficult to disentangle key processes such as exciton dissociation, charge-transfer (CT) state formation, and free-charge generation. To overcome these limitations, this study [1,2] employs dilute donor/acceptor model systems, which provide a significantly simplified and well-controlled morphology. These systems allow direct probing of charge-generation pathways by minimizing phase-separation and reducing structural ambiguity compared to conventional BHJs. Preliminary measurements across multiple NFA/donor systems reveal that charge-generation efficiency strongly depends on the interplay between film morphology, energetic offsets, and the donor/acceptor doping ratio (see figure below). Additionally, aggregation-driven charge generation is examined in selected NFA blends to evaluate how molecular packing influences early-time photophysics. These results highlight the importance of understanding morphology-dependent and aggregation-induced charge generation mechanisms in simplified NFA architectures, offering new insights that can guide the rational design of next-generation high-efficiency OPV materials.

References

Juhui Oh et al., Achieving excellent charge balance and transport in low-donor bulk heterojunctions for high performance semitransparent organic photovoltaics. J. Mater. Chem. A, 2025, 13, 30084–30094.

Soyeong Jeon et al., Critical Role of Non-Fullerene Crystalline Domains inStabilizing Charge Separation in Bulk HeterojunctionOrganic Solar Cells. Adv. Energy Mater. 2025, 15, 2501633.

Composition-dependent modulation of electrical transport in $WO_3/CuWO_4$ heterostructures induced by quinoline derivative incorporation

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Understanding and controlling charge transport in mixed metal oxide systems is essential for the development of functional electronic and optoelectronic devices. In this work, we investigate the effect of a quinoline derivative incorporation on the electrical transport behavior of $WO_3/CuWO_4$ heterostructures with distinct compositions (90%/10% and 50%/50%).

Current-voltage measurements reveal that the electrical response strongly depends on both composition and quinoline presence. The WO_3-rich sample exhibits a quasi-ohmic but nonlinear behavior, indicating trap-limited or barrier-influenced transport. Upon quinoline incorporation, a significant increase in current is observed, accompanied by enhanced nonlinearity, suggesting modification of interfacial states and charge injection barriers.

In contrast, the quasi-equimolar $WO_3/CuWO_4$ sample displays a more linear, near-ohmic response. Quinoline addition leads to a uniform increase in current under both dark and illuminated conditions, indicating an overall enhancement of bulk or interfacial conductivity rather than a selective modification of transport regimes.

These results demonstrate that the quinoline derivative acts as an effective electronic modulator, with its impact governed by the oxide composition. The findings highlight the role of organic molecules in tuning charge transport mechanisms in mixed oxide systems, opening new possibilities for interface engineering in hybrid electronic materials.

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References
Escaliante, L. C., Azevedo Neto, N. F., Mendoza, H. E., Xiao, C., Kandel, R., da Silva, J. H. D., & Osterloh, F. E. (2025). WO3/CuWO4 Ratio Controls Open-Circuit Photovoltage and Photocurrent in Type II Heterojunction Solar Fuel Photoelectrodes. ACS Applied Energy Materials, 8(5), 3198-3208.

Development and Characterization of MoS_2/PEDOT:PSS Thin Films with Potential Application in VOC Sensors

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Simple and engineered hybrid thin films of MoS_2/PEDOT:PSS were developed to investigate their performance as resistive sensors for volatile organic compounds (VOCs). Morphological characterization by profilometry and scanning electron microscopy confirmed the formation of continuous and homogeneous films with an average thickness of approximately 30 nm, evidencing nanometer-scale control of the deposition process. The chemical and structural integrity of the bilayer system was verified by Raman spectroscopy, while the optical properties, analyzed by UV–Vis–IR spectroscopy, demonstrated high transparency in the visible region and a combined contribution of both layers to the absorbance profile. Electrical measurements obtained from I–V curves revealed an increase in electrical conductivity compared to the isolated materials, as well as non-ohmic behavior, indicating a modification of the charge transport properties due to the formation of the MoS_2/PEDOT:PSS bilayer structure. In the sensing application, the device exhibited a significant electrical response to concentrations of 500 ppm of methanol and ethanol, both classified as VOCs. A clear distinction between the analytes was observed in both the response magnitude and the dynamic behavior, enabling differentiation between methanol and ethanol. The sensor presented a response close to 100% for methanol and approximately 60% for ethanol, with methanol also showing a faster response time of about 14 s, indicating a more efficient interaction with the active surface of the film. These results demonstrate that MoS_2/PEDOT:PSS bilayer films constitute a promising platform for the selective and distinguishable detection of VOCs.

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References
Almeida, L. F., Barcote, M. V. W., das Neves, M. F. F., Ferreira, M. S., Roman, L. S., Bassi, M. J., & Oliveira, C. K. (2025). Modeling the electrical conductivity of MoS_2 and PEDOT:PSS nanocomposites thin films obtained in an environmentally friendly system. Journal of Physics D: Applied Physics, 58(19), 195303.

Kumar, A., Tripathi, D., Rawat, R. K., & Chauhan, P. (2024). Hybrid MoS_2/PEDOT:PSS sensor for volatile organic compounds detection at room temperature: Experimental and DFT insights. ACS Applied Nano Materials, 7(23), 27599–27611.

Dielectric Characterization of Electrospun PVDF-based Nanocomposites with Graphene Nanoplatelets

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In the light of human machine interfaces and the increasing integration of artificial intelligence (AI), the growing demand for long-lasting autonomous electronic systems has highlighted the technological bottleneck imposed by conventional batteries, which are traditionally limited by their lifespan, the need for periodic maintenance, and the environmental and health impacts associated with their disposal [1]. In this context, self-powered systems such as piezoelectric nanogenerators (PENGs) and triboelectric nanogenerators (TENGs) have emerged as promising technologies for converting mechanical energy into electrical energy, reducing reliance on batteries and contributing to energy sustainability. These systems enable the development of low-environmental-impact electronic devices that can be integrated into intelligent applications, such as environmental and medical remote monitoring, wearable devices, and Internet of Things (IoT)-based systems [2]. Thus, this work proposes the investigation of dielectric properties and electrical relaxation mechanisms under AC regime in fibrous nanocomposites obtained via electrospinning and composed of poly(vinylidene fluoride) (PVDF) containing different weight fractions (wt%) of graphene nanoplatelets (GNP), aiming at the development of electroactive layers for PENGs, TENGs, and hybrid piezoelectric–triboelectric nanogenerators (PT-HNGs). The electrospun nanofibrous mats were characterized by Scanning Electron Microscopy (SEM) and Impedance Spectroscopy (EIS) to determine the response profile of the imaginary impedance (Z″) and real impedance (Z′), as well as the figures of merit associated with the electrical output performance of each nanocomposite as a function of the incorporation of additives into the polymer matrix.

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References
Hussain, S. Z. et al. Piezoelectric-Triboelectric Hybrid Nanogenerator for Energy Harvesting and Self-Powered Sensing Applications. Small 21, 2504626 (2025).

Dai, Y. et al. High-Performance Triboelectric Nanogenerator Based on Electrospun Polyvinylidene Fluoride-Graphene Oxide Nanosheet Composite Nanofibers. Energy Technology 11, 2300426 (2023).

Effect of deposition technique on the polyaniline-based thin films for PTMs detection

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Polyaniline (PAni) thin films are widely studied for sensor applications; however, the influence of sample fabrication on film reproducibility and electrical stability under aqueous conditions remains poorly understood [1] . In this work, we present a comparative analysis of PAni and PAni with Carbon Nanotubes (CNT) thin films prepared by Drop-casting (Dc) and Spray- coating (Sp), focusing on the time-dependent electrical response under exposure to mercury(II) chloride (HgCl 2). The thin films were deposited onto interdigitated gold electrodes and their reproducibility was evaluated by current–voltage measurements in triplicate. UV–Vis and Ra- man spectroscopy were performed and enabled analysis of the samples' optical and vibrational behavior [2,3] . Detection analysis was carried out by current–time measurements at a constant voltage of 1 V for 60 minutes, comprising 30 minutes with no analyte followed by 30 minutes after the addition of each analyte separately: ultrapure water as baseline and aqueous HgCl2 . A marked difference in film reproducibility between deposition techniques was observed, with films deposited by Dc showing a coefficient of variation of 13% compared to 68% for films fabricated by Sp. Regarding detection, the electrical current of PAni prepared by Dc exhibited distinct behaviors when the film was exposed to the analytes, suggesting an interaction with metal ions, in contrast to the test performed with PAni prepared by Sp. Incorporation of CNTs into the film further altered the electrical behavior: film conductivity increased, but an increase in the level of electrical noise under the same conditions was observed. The results demonstrate that the PAni deposition technique influences both the reproducibility of film fabrication and the electrical detection response to analytes in aqueous media. Incorporation of CNTs does not necessarily improve the robustness of the detection signal, despite enhancing the conductivity of the PAni film.

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References

M.A. Deshmukh, M.D. Shirsat, A. Ramanaviciene and A. Ramanavicius, Crit. Rev. Anal. Chem. 48, 293 (2018).

M. Abdolkarimi-Mahabadi, A. Bayat and A. Mohammadi, Theor. Exp. Chem. 57, 191 (2021).

R. Mažeikiene, G. Niaura and A. Malinauskas, J. Solid State Electrochem. 23, 1631 (2019).

Fabrication of an Amplifier Circuit Using Liquid Crystalline Organic Semiconductor Thin Film Transistors

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Organic semiconductors are expected to be applied in wearable sensors due to their high flexibility. Also, there is a need for circuits of amplifying the weak signals obtained from these sensors. Previously reported organic thin film transistor (OTFT) based amplification circuits have generally used vapor-deposited films, such as DNTT, as the active layer of OTFTs [1]. In this study, we report the fabrication of an amplification circuit in which the active layer was formed by solution process using liquid crystalline organic semiconductor 2-decyl-7-phenyl-[1]benzothieno[3,2-b][1]benzothiophene (Ph-BTBT-10). It exhibits the highly ordered liquid crystal phase, and by utilizing its liquid crystallinity, it has been reported to enable the formation of uniform polycrystalline thin films and OTFTs with high mobility above 1cm^2/Vs. [2].

The fabricated amplifier circuit consists of a current mirror circuit, a differential amplifier circuit, and a common-drain circuit. All of them are composed of p-type transistors. The transistors were fabricated on a glass substrate using bottom-gate and bottom-contact structure. Pentafluorobenzenethiol(PFBT)-treated Au was patterned by lift-off process to form the source and drain electrodes. Al_2O_3 (30 nm) and poly(vinyl cinnamate) (PVCi) (100 nm) were used as the gate insulator layer [3]. The active layer was formed by spin-coating a polystyrene-mixed Ph-BTBT-10 solution via liquid crystal phase and patterned by photolithography and oxygen plasma ashing. OTFTs fabricated using Al_2O_3/PVCi gate insulator showed the average mobility of 1.6 ± 0.64 cm^2/Vs and the average threshold voltage of 0.62 ± 0.40 V for 10 samples. The input-output voltage characteristics of the fabricated amplifier circuit exhibited a maximum gain of dV_{out}/dV_{in} = 2.1. These results demonstrate the successful operation of a solution-processed organic amplifier circuit using liquid crystalline Ph-BTBT-10, offering a promising approach for wearable sensor systems.

References

S. Elsaegh et al. IEEE JOURNAL OF SOLID-STATE CIRCUITS, 55, 9 (2020).

H. Iino et al. Nature Communications, 6, 6828 (2015).

I. Suzuki et al. Physica Status Solidi (a), 220, 2300281 (2023).

Fluorene-Decorated Donor–Acceptor Emitters with TADF and High Hole Mobility for Solid-State Picric-Acid Sensing and Sky-Blue OLEDs

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Two donor–acceptor–donor emitters incorporating four fluorene units, N,N,N′,N′-tetrafluoren-2-yl-4,4′-diaminobenzophenone (FABP) and its ethyl-substituted analogue (EFABP), were synthesized and systematically investigated with respect to their photophysical, charge-transport, and sensing properties. In rigid, non-polar host matrices, FABP exhibits dual emission comprising thermally activated delayed fluorescence (TADF) and room-temperature phosphorescence, indicating the coexistence of emissive singlet and triplet decay pathways. Substitution of ethyl groups on the fluorene moieties suppresses the phosphorescent contribution, resulting in emission dominated by delayed fluorescence. Thermal treatment reveals the presence of multiple emissive conformers, which influence the excited-state behavior and spectral characteristics. When molecularly dispersed in an inert polymer matrix, EFABP achieves a photoluminescence quantum yield of up to 44%. In the solid state, the material demonstrates high hole mobility approaching 10-3 cm2 V-1 s-1 at elevated electric fields. The films exhibit pronounced luminescence quenching in the presence of picric acid, indicating potential utility in nitroaromatic sensing. Furthermore, EFABP functions as a sky-blue emitter in organic light-emitting diodes, affording low turn-on voltage and a maximum external quantum efficiency of 16.6%.

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References
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Gas Sensing Properties of Polythiophenes and Fullerene Derivatives

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Fullerenes and polythiophenes are materials widely used in organic electronics due to their properties. Polythiophene derivatives exhibit relatively high electrical conductivity and excellent chemical stability, while fullerene derivatives are known to be efficient charge acceptors. These properties provide these materials with significant potential for application in the field of gas sensors, devices commonly used for safety monitoring and quality control by detecting the presence of unwanted compounds. The materials used in this work were OPCBMMB, a fullerene derivative, and P3HT and P3OT, both polythiophene derivatives. These materials were studied as blends of OPCBMMB/P3HT and OPCBMMB/P3OT. The aim of this work is to evaluate the applicability of these materials as gas sensors by monitoring their electrical response when exposed to a saturated atmosphere of different analytes. The blends were prepared using chloroform as the solvent, at a concentration of 1.0 mg mL^{-1} and with a 1:1 mass ratio of fullerene to thiophene. The films were fabricated using the drop-casting and Langmuir–Schaefer techniques.The results observed for the blends are similar to those obtained for pristine thiophene-based materials, as reported in previous studies, suggesting a dominance of the thiophene component over the fullerene. This behavior may be attributed to differences in molecular weight between the materials, leading to a higher proportion of thiophene molecules in the mixed films. In addition, the analysis of the coefficient of variation allowed the reproducibility of the gas response to be evaluated for each exposure cycle.

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References

L. K. M. Roncaselli et al., “Influence of solvents on the morphology of Langmuir and Langmuir-Schaefer films of PCBM and PCBM-based oligomers and polymers,” Phys. Chem. Chem. Phys., vol. 24, no. 20, pp. 12442–12456, 2022, doi: 10.1039/d1cp05408b.

Simõis, André V. S., et al. “Fabrication and Characterization of Poly(Fullerene) Thin Films for Gas Sensors.” Polymer International, no. February, Sept. 2024, https://doi.org/10.1002/pi.6698.

Grain-Boundary-Driven Stochastic Oxide Junction in 2D SnSe Enables Dual Electrical-Optical PUFs

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Introducing scalable physical entropy into solid-state platforms is a key challenge for secure hardware systems. Here, we present a dual-mode physically unclonable function (PUF) based on grain-boundary-induced oxidation in two-dimensional (2D) tin selenide (SnSe) multilayers. Photo-oxidative activation selectively induces oxidation along the grain boundaries, Inducing the phase transition of SnSe into tin dioxide (SnO_2). As a result, spatially random SnSe/SnO_2 oxide junctions are formed without the need for lithographic patterning. This guided disorder transforms uniform polycrystalline films into high-entropy architectures, where nanoscale variations in composition and conductivity arise from the intrinsic microstructure. Electrical measurements reveal device-to-device variability driven by localized junction asymmetry, while optical excitation independently modulates photocurrent responses, enabling dual electrical–optical challenge–response behavior. At optimized oxidation duration, the system achieves maximal entropy and low inter-mode correlation, yielding cryptographically robust and mode-orthogonal keys. Beyond fundamental interest, our results demonstrate a template-free, material-intrinsic strategy for engineering multi-dimensional entropy in 2D semiconductors. This approach offers a scalable pathway toward secure and reconfigurable hardware applications and further opens opportunities for next-generation security platforms, advanced Internet of Things (IoT) devices, and adaptive optoelectronic systems.

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References
Lee, D. H., Han, Y., Woo, G., Koo, R. H., Shin, H., Cho, J., ... & Yoo, H. (2025). Over 1011-fold variability for a base-12 PUF using particle-damaged graphene. Device, 3(12).

Green Synthesis of 2D Conjugated Polymer Networks via Metal-Free Click Chemistry for High-Performance OECTs

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We present a sustainable strategy to construct two-dimensional (2D) conjugated polymer networks for organic electrochemical transistor (OECT) applications. A fluorinated bithiophene-based polymer was synthesized using N-butylpyrrolidinone (NBP) as a green solvent. Azide-functionalized side chains were then introduced via post-polymerization modification, followed by strain-promoted azide–alkyne cycloaddition (SPAAC) with bis-DBCO series to form a covalently crosslinked network.

This metal-free click reaction proceeds under mild conditions, enabling efficient network formation while preserving the conjugated backbone. The resulting material combines enhanced ionic transport from PEG segments with efficient electronic conduction from the conjugated framework, delivering balanced mixed conduction and improved stability.

This work demonstrates a green and versatile approach to designing 2D conjugated networks, offering strong potential for high-performance OECT applications.

References

Kimpel et al., Sci. Adv. 11, eadv8168 (2025)

Hybrid GO-AuNPs-Silsesquioxane Nanocomposites: Synthesis, Characterization, and Electrochemical DNA Biosensing

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Random silsesquioxanes (SSQs) are versatile inorganic-organic hybrid materials featuring a siloxane (Si-O-Si) framework with the general formula (RSiO1.5). The incorporation of organofunctional groups within these structures enables the stabilization and morphological control of metallic nanoparticles (MNPs). In this work, graphene oxide (GO) was integrated with gold nanoparticles (AuNPs) stabilized by pyridinium-functionalized SSQ via electrostatic interactions, yielding a high-performance GO-AuNPs-SSQ nanocomposite. XRD analysis confirmed the hybrid's crystalline integrity, identifying the face-centered cubic (fcc) structure of AuNPs and the (002) graphitic plane of GO within the silica network. TEM imaging revealed predominantly spherical AuNPs (7.05 nm) successfully anchored onto the GO sheets, while UV-Vis spectroscopy corroborated the synthesis via the surface plasmon resonance (SPR) band at 527 nm. Zeta potential measurements indicated a high positive surface charge (+45.7 mV), attributed to effective surface polarization and the robust anchoring of functionalized nanoparticles. These results, supported by molecular dynamics, demonstrate that the high surface potential prevents agglomeration and ensures material stability. The nanocomposite was applied to modify screen-printed carbon electrodes (SPCE) for the *in situ* electrochemical quantification of the genome of plant growth-promoting bacteria. The optimized biosensor exhibited a sensitivity of 9.339%/log{genome}, with detection (LOD) and quantification (LOQ) limits of 1.084 and 1.279 ng µL-1, respectively. Furthermore, the device demonstrated high selectivity, successful detection in real samples, and remarkable long-term stability of 21 weeks. This stable, carbon-based hybrid architecture presents significant potential for advanced (bio)sensing applications in sustainable agriculture.

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References

[1] Zahrebelnei F., et al. Chemosensors 12, 259 (2024).

[2] Zahrebelnei F., et al. Talanta 286, 127484 (2025).

Impact of the process conditions for the deposition of the source and drain contacts on the contact resistance in organic thin-film transistors

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We investigate how process parameters during gold (Au) source/drain deposition affect the contact resistance in inverted coplanar organic thin-film transistors (TFTs). By varying the substrate temperature (20-150 °C) and deposition rate (0.3-3.0 Å/s), a clear correlation between deposition conditions, contact morphology, and electrical performance is identified. TFTs were fabricated in an inverted coplanar architecture with Au source/drain electrodes. Atomic force microscopy shows that low substrate temperatures combined with high deposition rates produce smooth, fine-grained Au films with low surface roughness (~1.2 nm), whereas high substrate temperatures and low deposition rates yield larger grains and increased roughness (up to ~7.4 nm). Electrical characterization using the transmission line method shows that smooth contacts exhibit high contact resistance (up to 1 kΩcm), while rough contacts yield substantially reduced values (down to 200 Ωcm). This counterintuitive trend indicates that increased surface roughness enhances charge injection, likely due to an enlarged effective injection area at the Au/semiconductor interface. These results contrast with previous findings for aluminum gate electrodes, where low surface roughness is required for optimal subthreshold swing, highlighting the need for interface-specific optimization in organic TFTs. The findings highlight the critical role of deposition conditions in tailoring contact morphology and optimizing device performance in organic TFTs.

References

M. Noda et al., J. SID, 19, 316 (2011).

U. Zschieschang et al., Adv. Funct. Mater., 30, 1903812 (2020).

M. Geiger et al., Adv. Mater. Interfaces, 7, 1902145 (2020)

Industrial Upscaling of Organic Photovoltaic Devices: Analyzing the Transition from Stepwise Regime to Large-Area Continuous R2R Processing

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The successful transition from laboratory protocols to large-scale industrial manufacturing regimes is one of the primary challenges for the commercial viability of organic photovoltaic (OPV) devices. This upscaling process introduces complexities inherent to deposition dynamics, interface stability, and multi-layer integration [2]. While lab-scale roll-to-roll (R2R) processing predominantly operates in a stepwise (semi-continuous) regime, allowing for isolated optimization of each functional layer, industrial production requires the systemic synchronization of all deposition stages within a single manufacturing run. In this scenario, the spreading, drying, and wetting behavior of functional inks become interdependent under a unified and constant line speed. This study evaluates the processing conditions for upscaling OPV printing, comparing the laboratory scale (110 mm web width) with the industrial scale (500 mm web width). The results evidence that the parameters established in the laboratory present limitations, requiring further refinement to ensure operational stability under a fully continuous regime. To mitigate the discrepancies between these regimes (as the continuous system operates at a constant speed for the simultaneous deposition of all layers) most operational conditions were adjusted. These modifications aim to compensate for the kinematic asymmetry between scales, given that industrial processing occurs on a machine with an average operating speed 5 times higher than that used in the laboratory, while the print head dimensions are 4.5 times larger. The adaptations performed proved crucial in ensuring device functionality and mitigating efficiency losses associated with area scaling. Mastering these variables establishes the foundation for developing more robust and reproducible OPV manufacturing methods at an industrial scale.

References

Yourui Zang, et al., Materials Today Energy, v. 54, art. 102150, (2025).

R. Adel, et al., Solar Energy Materials and Solar Cells, v. 245, art. 111852, (2022).

Y. Galagan, et al., Chemical Engineering and Processing, v. 50, p. 454-461, (2011).

Inkjet-printed graphene-based electrodes for flexible organic devices on biodegradable substrates

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The growing demand for flexible and sustainable electronic systems has stimulated the development of materials compatible with low-cost and scalable fabrication. This work investigates inkjet-printed graphene-based electrodes integrated into flexible organic electronic platforms on biodegradable substrates.

Graphene inks were formulated using terpineol to achieve suitable rheological properties for stable drop-on-demand deposition. Electrodes were printed using a Dimatix DMP-2850 system onto polylactic acid and nanocellulose substrates, enabling precise control of geometry and thickness. Printing parameters, including drop spacing and substrate temperature, were optimized to ensure film uniformity and electrical continuity.

The electrodes were evaluated regarding mechanical flexibility, adhesion, and stability under bending. Electrical properties were measured by four-point probe, while morphology was analyzed by atomic force microscopy, correlating microstructure with conductive performance.

Results indicate that graphene electrodes exhibit competitive electrical behavior and mechanical robustness, while maintaining compatibility with biodegradable substrates, demonstrating their potential for sustainable flexible organic devices.

Acknowledgements
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References

SECOR, E. B.; PRABHUMIRASHI, P. L.; PUNTAMBEKAR, K.; GEIER, M. L.; HERSAM, M. C. Inkjet printing of high conductivity, flexible graphene patterns. Journal of Physical Chemistry Letters, v. 4, n. 8, p. 1347–1351, 2013. American Chemical Society.

SHI, K.; HU, M.; HUANG, P. Study on Adhesion Force of Graphene under Cylinder–Plane Contact. Lubricants, v. 11, n. 3, 2023. MDPI.

EZZAT, Markos; RASHED, Ahmed E.; SABRA, Sally A.; et al. Fully inkjet-printed graphene/gold nonenzymatic biosensor for glucose detection. Materials Today Communications, v. 37, p. 107549, 2023.

Kinetic Monte Carlo modelling of organic optoelectronic devices for optical communication

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Organic light emitting diodes (OLEDs) and photodiodes (OPDs) present compelling alternatives to their inorganic counterparts in optical communication owing to their spectral tunability and the absence of toxic or resource critical elements. A possible downside could be the low charge-carrier mobility of organic semiconductors, but when high biases are applied one can profit from the strong field enhancement of the mobility. Current modelling of organic optoelectronic devices predominantly relies on rate equation or drift-diffusion approaches, which are insufficient in describing the coupled charge transport and excitonic processes occurring at the molecular up to the device scale. Mechanistic Kinetic Monte Carlo (kMC) simulations can capture all these processes at all relevant spatial and time scales, and are therefore perfectly suitable to explore the fundamental mechanisms that ultimately constrain data rates and device performance. In this work, we employ kMC simulations to analyse the reported transient behaviour of an OLED [1] and an OPD [2] driven by a sequences of voltage or optical pulses, respectively. By systematically varying the repetition rates and key device/material parameters, we study their impact on the luminescence and photocurrent transients, as well as on the spatiotemporal evolution of excitons and charges inside the devices. We find that the bandwidth in both devices can be greatly reduced by increasing the bias voltage, demonstrating the feasibility of using OLEDs and OPDs in optical communication with speeds that can compete with their inorganic analogues.

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References

K. Yoshida et al., Nature 621, 746 (2023).

S. Ullbrich et al., J. Phys.Chem. Lett. 8(22), 5621 (2017).

Material- and System-Level Characterization of Metal Alloy Thin Films for Near-Field Magnetic EMI Suppression in Smart Electronics

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Near-field magnetic coupling is a major source of electromagnetic interference (EMI) in compact smart devices, where densely integrated circuits, power lines, and high-speed interfaces are closely packed. Metal alloy thin films are promising candidates for lightweight and compact EMI shielding, but their effectiveness cannot be fully described by conventional far-field shielding metrics alone [1. 2]. In this study, we propose a dual evaluation framework for assessing the near-field magnetic shielding performance of metal alloy thin films using both standardized material-level measurements and system-level validation with a Raspberry Pi platform. Loop-antenna and microstrip-based test structures are employed to quantify the intrinsic suppression characteristics of the thin films, while the Raspberry Pi serves as a practical smart-device model for identifying magnetic hot spots under operating conditions. This approach enables direct correlation between intrinsic shielding behavior and practical noise reduction on real hardware, providing an effective platform for optimizing metal alloy thin films for next-generation smart-device EMI shielding applications.

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References

A. Khan, et. al., J. Alloys and Compounds, 1064, 187955, 2026

X.-Y. Wang, et al., Materials Today Physics, 23, 100644, 2022

Materials for Quantum Information Science

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Quantum Information Science (QIS) uses fundamental quantum mechanical phenomena such as superposition and entanglement of quantum states for applications in a wide range of fields including sensing, communications, and computing [1]. The S = 1/2 ground state of [Cr7Ni] wheels, makes these units ideal for applications in supramolecular assemblies as quantum bits (qubits). The first examples of such heterometallic rings, [nPr2NH2][Cr7MII(μ-F)8(O2CtBu)16], were reported in 2003 [2], and since then the [Cr7Ni] units were featured in the design of various multi-ring complexes including the nanoscopic [Pd12[Cr7Ni-Py2]24] cage [3]. The molecular materials for application in QIS and their properties will be presented with the target featuring two [R1R2NH2][Cr7Ni(μ-F)8(O2CtBu)16] units connected with a π-functional linker.

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References

Wasielewski, M.R., et al., Exploiting chemistry and molecular systems for quantum information science. Nature Reviews Chemistry, 2020. 4(9): p. 490-504.

Larsen, F.K., et al., Synthesis and Characterization of Heterometallic {Cr7M} Wheels. Angewandte Chemie International Edition, 2003. 42(1): p. 101-105.

Ferrando-Soria, J., et al., Controlled Synthesis of Nanoscopic Metal Cages. Journal of the American Chemical Society, 2015. 137(24): p. 7644-7647.

Mechanistic modelling of exciton-polaron quenching in thermally activated delayed fluorescence emitters

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A major source of efficiency loss in organic light emitting devices (OLEDs) are so-called ‘quenching’ losses, which scale with the density of charge carriers present in the device. Exciton quenching occurs when charged molecules (holding either a hole or electron) can absorb excitonic species which would otherwise have emitted light. This reduces device efficiency and contributes towards device degradation. Potentially, the role of quenching can be reduced when using thermally-activated fluorescent (TADF) emitters, with emissive lifetimes that can be much shorter than that of phosphorescent emitters. In previous studies [1,2], quenching in TADF-based devices has been studied using a phenomenological (rate-equation) model. However, the various approximations that are made using such approaches limit their applicability and do not allow a comparison with results of first-principles (quantum-chemical) methods. Here, we develop a mechanistic description of the efficiency loss due to TPQ for the prototypical blue-green TADF emitter material DMAC-TRZ, by analyzing the current-density dependence of the time-resolved photoluminescence (TRPL) of single-layer hole-only (see Figure 1) and electron-only devices. The system is modelled using kinetic Monte Carlo simulations to analyse the observed quenching. For hole-only devices (see Figure 1), the delayed component of the TRPL is found to be most strongly affected, indicating that triplets are quenched more strongly than singlets. The KMC analysis is used to obtain the rate of Dexter-type triplet-hole quenching. The validity of the approach is demonstrated by making a comparison with the quenching in films in which DMAC-TRZ is blended with a high-energy gap spacer material.

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References
A. Sandanayaka et al. J. Phys. Chem. C 119, 14, 7631–7636 (2015)

Hasan, M. et al. Nat Commun 13, 254 (2022)

Memristive self-assembled multilayers of octahedral ruthenium complexes with non-innocent redox-active ligands

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The advance of artificial intelligence (AI) represents the largest market opportunity in the history of humankind, estimated to be anywhere between USD 3.5 and 5.8 trillion.1 However, it also represents a grave environmental challenge. As a typical example, hundreds of millions of daily queries on ChatGPT can cost around 1 GWh each day, equivalent to the daily energy consumption for about 33,000 U.K. households. This trend is unsustainable, and new approaches are needed now. The fundamental limitation of modern computing is the rate of data transfer between a processing unit and memory, known as the von Neumann bottleneck.2 This data transfer not only limits computational speed, but is also highly energy-intensive. To overcome this bottleneck there is a global demand for new technologies for brain-inspired, neuromorphic, computing within memory. Memristors are one of the most promising technologies for achieving in-memory computation. Short for “memory resistors”, memristors are considered the fourth fundamental passive circuit element, alongside resistors, capacitors, and inductors.3 However, in contrast to traditional volatile memory technologies like RAM, which lose data when power is lost, memristors are a class of non-volatile memory, whose resistive state is maintained even when no external power is applied. In this work, we demonstrate a new class of redox-active, octahedral ruthenium azopyridine compounds with a host of different surface anchoring groups compatible with CMOS-compatible electrodes. I will present the synthesis, in-depth NMR and EPR studies in combination of crystallographic analysis to elucidate the structure-function-property relationship of these complexes and their application in scalable, ordered, self-assembled molecular multilayers when in contact with the electrodes stated above.

References

M. Chui, M. et al. The economic potential of generative AI. (2023).

D. Ielmini, et al. In-memory computing with resistive switching devices. Nature Electronics 1, 333-343 (2018).

S. Goswami, et al. Nature Materials 16, 1216-1224 (2017).

Multi-heterojunctioned plastics with high thermoelectric figure of merit

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Conjugated polymers promise inherently flexible and low-cost thermoelectrics for powering the Internet of Things from waste heat. Their valuable applications, however, have been hitherto hindered by the low dimensionless figure of merit (ZT). Here we report high-ZT thermoelectric plastics, which were achieved by creating a polymeric multi-heterojunction with periodic dual-heterojunction features, where each period is composed of two polymers with a sub-ten-nanometre layered heterojunction structure and an interpenetrating bulk-heterojunction interface. This geometry produces signifcantly enhanced interfacial phonon-like scattering while maintaining efcient charge transport. We observed a signifcant suppression of thermal conductivity by over 60 percent and an enhanced power factor when compared with individual polymers, resulting in a ZT of up to 1.28 at 368 kelvin. This polymeric thermoelectric performance surpasses that of commercial thermoelectric materials and existing fexible thermoelectric candidates. Importantly, we demonstrated the compatibility of the polymeric multi-heterojunction structure with solution coating techniques for satisfying the demand for large-area plastic thermoelectrics, which paves the way for polymeric multi-heterojunctions towards cost-efective wearable thermoelectric technologies.

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References

Nature 2024, 632: 528-535.

Nanostructured Films and Nanofibers Using Low-Bandgap Polymer-Based Sensitive Surfaces to Detect VOCs

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The growing concern over the health effects of air pollutants, such as volatile organic compounds (VOCs), has motivated the development of sensitive gas sensors. Conductive polymers (CPs) have emerged as promising materials for these compounds due to their low cost, high sensitivity, and room-temperature operation. Among CPs, low-bandgap polymers have been evaluated for gas sensing due to their low-energy electronic structure, which may facilitate significant and detectable changes in conductivity upon interaction with gas molecules [1]. In this work, chemiresistive sensors based on the low bandgap cyclopentadithiophene (CPDT):diketopyrrolopyrrole (DPP)-based polymer (PCPDTDPP_C12) are proposed. For comparison, two approaches were selected: Thin films sensors were fabricated using the Langmuir-Schaefer technique, and polyvinylidene fluoride (PVDF) fibers were prepared by the electrospinning technique and posteriorly a PCPDTDPP_C12 solution was dripped onto the fibers. Both devices were prepared onto silicon slides and interdigitated electrodes of gold (IDE_Au) substrates. The devices were morphologically characterized by Scanning Electron Microscopy (SEM) and electrically characterized by direct current versus voltage (I vs V) measurements, from which conductivity and resistance were estimated, showing one order of magnitude values in favor of the decorated fibers. For gas sensing, the sensors were evaluated through exposure cycles to toluene and tetrahydrofuran (THF) in a saturated atmosphere. The devices exhibited a decrease in the current under exposure to both VOCs, which indicates an increase in sensor resistance. The higher response was observed in THF. Additionally, the decorated fibers exhibited a higher response over the thin films, which can be related to the higher surface area derived from the nanofibers [2]. Overall, the PCPDTDPP_C12 polymer exhibited a sensitivity to both VOCs, which indicates their potential as a sensitive surface in sensing device.

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References

Wang, Z. et al. Highly Sensitive Field-Effect Ammonia/Amine Sensors with Low Driving Voltage Based on Low Bandgap Polymers. Advanced Electronic Materials 4, 1800025 (2018).

Lang, K. et al. Nanofibers enabled advanced gas sensors: A review. Advanced Sensor and Energy Materials 3, 100093 (2024).

Nanostructured Polyaniline Films Prepared by the Langmuir-Schaefer Technique for the Development of Sensing Platforms

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Nanostructured platforms based on conducting polymers have attracted interest for electrochemical sensors due to their tunable electrical properties, high surface area, and molecular-level organization [1]. Among them, polyaniline emeraldine salt (PANI-ES) stands out for its redox activity, stability, and ease of preparation. The Langmuir-Schaefer technique enables the formation of organized ultrathin films with a controlled architecture, thereby favoring interactions between the sensing layer and target molecules. In this work, nanostructured PANI-ES films were prepared by Langmuir-Schaefer deposition to develop an electrochemical sensing platform. Methylene Blue (MB) was selected as a model analyte and electrochemical probe due to its environmental relevance and well-defined redox behavior [2]. In the first step, the interactions between PANI-ES and MB were investigated in Langmuir films. PANI-ES π-A isotherms in the absence and presence of MB showed a shift toward larger molecular areas, indicating polymer-dye interactions in the gaseous and liquid-expanded phases. Then, five-layer LS films were deposited onto quartz and ITO substrates, monitored by UV-Vis spectroscopy, and evaluated by Cyclic Voltammetry (CV) and Differential Pulse Voltammetry (DPV). UV-Vis spectra and voltammograms showed characteristic features of PANI-ES and contributions attributed to MB, confirming the PANI-ES/MB system. The PANI-ES film exhibited a redox pair between −0.5 and +0.45 V, while MB showed a peak at approximately +0.25 V. After cleaning, MB readsorption was evaluated in a 1×10^{-6} mol L^{-1} solution for 10, 20, and 30 min. The 20-min interval resulted in the largest current increase and was selected for subsequent analyses, achieving a LOD below 10^{-7}mol/L. These results indicate that LS PANI-ES films are promising nanostructured platforms for electrochemical sensing beyond MB detection.

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References

A. Dube et al., Sustainable Materials and Technologies 43, e01264 (2025).

I. Khan, K. Saeed, I. Zekker, B. Zhang, A.H. Hendi, A. Ahmad, S. Ahmad, N. Zada, H. Ahmad, L.A. Shah, T. Shah and I. Khan, Water 14, 242 (2022).

Near-/Far-Field Evaluation of Conducting–Magnetic Thin Films for Radiated-EM Energy Mitigation in Smart Hybrid Electronics

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Radiated electromagnetic (EM) energy in smart hybrid electronics is intensified by dense clocking, switching power conversion, and wireless co-site operation. We evaluate Ag/Ni–Cu conducting–magnetic thin films as lightweight mitigation layers using a coupled far-/near-field protocol. Far-field shielding effectiveness is measured in the X-band with a WR-90 waveguide fixture and compared with Schelkunoff-theory predictions to validate the dominant response and assess fixture-inclusive deviations. Near-field performance is quantified using IEC 62333-2 metrics, including transmission-path attenuation (Rtp) and intra-/inter-decoupling ratios (Rda and Rde), enabling geometry-consistent ranking over a broad band. The films provide stable X-band shielding and strong transmission-path attenuation at sub-micrometer thickness, while inter-decoupling shows band-dependent crossover behavior relative to magnetic reference sheets. The framework offers band-selective integration guidance for smart hybrid electronics.

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References

M. Peng, F. Qin, J. Appl. Phys., 130, 225108 (2021)

A. J. McDowell, T. H. Hubing, IEEE Trans. Electromagn. Comp, 56, 1711 (2014)

T. Arakawa, et al., IEEE Trans. Electromagn. Comp., 65, 1037 (2023)

On the importance of reduced interpenetration of donor-acceptor interfaces in light harvesting capacitors: a comparison of small molecule vs. polymeric acceptor materials

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Light harvesting capacitors (LHCs) are photovoltaic devices in which the electrodes and the active layer are separated by an insulating film, preventing the direct extraction of photogenerated charges [1]. Instead, positive and negative charges accumulate within the donor and acceptor materials, forming an internal dipole that polarizes the active layer. This polarization induces charge accumulation at the electrodes, generating a transient current through the external circuit until a new equilibrium is reached. When illumination ceases, charge recombination reduces the polarization, producing a reverse transient current. As a result, LHCs exhibit peaked transient currents under modulated illumination. In this work, we investigate multilayered LHC devices fabricated via Layer-by-Layer (LbL) polyelectrolyte self-assembly. As the electron donor, we employ Poly[3-(potassium-6-hexanoate)thiophene-2,5-diyl] (P3KHT), while for the acceptor we compare the performance of a small molecule and a macromolecular cationic derivative of perylene diimide (PDI). Device characterization was performed using time-resolved transient absorption and continuous-wave photoinduced absorption spectroscopy to probe internal charge photogeneration, while transient photocurrent measurements assessed the external current response. By fitting the photocurrent data with an analytical model based on the photophysical behavior of LHCs, the lifetimes of coherent nanodipoles were extracted. Our results show that although the polymer-based device exhibits lower absorption and charge generation than its small molecule counterpart, its overall performance is superior. This enhancement is attributed to reduced interpenetration at the donor-acceptor interface when using the macromolecular acceptor, which promotes more efficient formation of coherent dipoles.

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References
[1] J. B. Lima Filho et al., (2024) ACS Appl. Polym. Mater., 6: 8040

One-Pot Synthesis of Nanoarchitectured Thin Films Formed by Carbon Nanomaterials and Metal Nanoparticles Deposited on Silica Substrate for Optical Applications

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The use of carbon nanomaterials, such as graphene, has become more interesting due to its fantastic properties, allowing several applications[1]. Nanocomposites formed by carbon nanomaterials and metal nanoparticles (NPs), may present different and new properties due to the interaction between their constituents, thus creating new materials[2]. These NCs have the advantage of a high surface/volume ratio, improved optical properties and being considered as an alternative to overcoming the limitations of conventional materials[3]. The present work aimed at the synthesis and characterization of thin films of mono/bimetallic NPs and nanocarbon materials on silica substrate, prepared at the same time in a single step synthesis route. As a substrate, silica coverslips previously cleaned and treated with piranha solution were used. Coverslips were immersed in a toluene solution containing (3-aminopropyl)trietoxysilane (APTES) together with the respective metallic salts (Ag, Cu and Ag+Cu), and with expanded polystyrene (EPS), remaining under heating at 60 °C for 3 hours. After this first step, the reduction of metallic ions were made by heating in a muffle furnace at 350 °C for 1 hour. At the end of the process, films were characterized by electron spectroscopy of absorption (UV-Vis), X-ray diffraction (XRD), Raman spectroscopy (Raman), scanning electron microscopy (SEM) and transmission electronic microscopy (TEM) and in high resolution TEM (HRTEM). NPs were formed in different phases: XRD and Raman spectroscopy showed the presence of metal Ag NPs and copper oxide structures. SEM showed the formation of homogeneous films, with some agglomerates associated with amorphous carbon and organized 2D structures. TEM and HRTEM images showed the presence of spherical NPs. The presence of carbon, both amorphous and crystalline, evident in the samples, but not continuously through the entire film. As larger amounts of EPS were added, greater quantity of 2D structures were obtained.

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References

D. PONNAMMA, et al. Composites Part B: Engineering, 204, 108493, (2021).

C. Y. HSU, et al., Case Studies in Chemical and Environmental Engineering, 8, 100535

(2023).

A. GUERRAM, et. al., Journal of Cluster Science, 35, 2231-2242, (2024).

Performance Optimization of Environmental Sensors: Investigating Non-Fullerene Thin-Films for Enhanced Humidity Detection

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Precise monitoring of relative humidity (RH) is a critical requirement in advanced instrumentation, where atmospheric moisture levels directly influence the stability of food preservation, biochemical and industrial processes control. Unlike the detection of hazardous gaseous analytes, RH sensing is indispensable for maintaining the operational integrity of moisture-sensitive electronic devices and ensuring thermodynamic equilibrium in controlled environments. Consequently, there is an intensifying demand for sensing platforms characterized by high sensitivity, low-cost fabrication, and fast signal transduction[1]. In this context, organic semiconductors have emerged as promising materials due to their ability to interact with water molecules at room temperature, reversibly altering their electrical properties while allowing for solution-based processing[2]. The sensor architecture was explored through different deposition methodologies to optimize active layer morphology and electrode interface: Langmuir-Schaefer (LS), offering nanometric molecular control; drop-casting, for technical simplicity; and decorated nanofibers, aimed at increasing surface area to optimize adsorption and desorption kinetics. The devices were characterized through direct current (DC) electrical measurements, evaluating parameters such as relative response, stability, and reversibility. Regardless of the fabrication technique, a substantial enhancement in electrical current was observed upon exposure to water vapor, coupled with excellent reversibility. However, distinct morphological characteristics led to variations in the coefficient of variation between cycles. Additionally, the techniques also leads to a large coefficiente of variations between cycles, a phenonemon attributed directly to the distinct morphological characteristics of the thin films. The results demonstrate the potential of non-fullerene semiconductors for a new generation of high-performance environmental sensors.

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References

[1] DAI, J. et al. Preparation of organic-inorganic hybrid polymers and their humidity sensing properties. Sensors and Actuators B: Chemical, v. 242, p. 1108–1114, 2017.

[2] CHENG, P. et al. Next-generation organic photovoltaics based on non-fullerene acceptors. Nature Photonics, v. 12, n. 3, p. 131–142, 2018.

Performance Optimization of OFETs by Interface Functionalization with loosely packed Self-Assembled Monolayers

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Organic Field-Effect Transistors (OFETs) are the cornerstone of organic electronics, just as inorganic transistors are fundamental to all current electronics. The advantages of OFETs include low-cost, straightforward fabrication and versatility due to chemical tuning of the semiconductor material. The dielectric-semiconductor interface of an OFET is critical, as its chemistry influences the semiconductor's structure and charge carrier mobility, with a marked effect on device performance. In this work, we functionalize the dielectric and electrodes with surfactant self-assembled monolayers (SAMs) to study their improvement in device parameters [1]. Previous work by Miranda et al. [2] had shown that, under certain circumstances, alkyl chains of low-coverage surfactant SAMs may self-organize upon interacting with long-chain molecules. Thus, the idea was to investigate whether this van der Waals interaction between the monolayer molecules and the polymer side chains has any effect in devices based on poly(3-alkylthiophene), with alkyl chains with 6, 10 and 16 carbons (P3HT, P3DT and P3HDT, respectively). It has been found through electrical measurements that indeed the presence of a loosely packed dioctadecyldimethyl bromide (DOAB) monolayer enhanced device performance, with a much larger effect for longer side-chain polymers (~ 100x higher mobility for P3HDT vs. P3HT). For further insight, the self-assembled monolayers will have their molecular conformation characterized by nonlinear vibrational (SFG) spectroscopy [3]. Thus, this study has shown how to control the OFET performance through modifications of the semiconductor-dielectric interface, in particular by exploiting the polymer side chain-SAM interaction.

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References

[1] S. Casalini and C. Bortolotti, Chemical Society Reviews v. 46, p. 40–71 (2017)

[2] P. Miranda and V. Pflumio, Journal of the American Chemical Society v. 120, p. 12092–12099 (1998)

[3] A. Lambert and P. Davies, Applied Spectroscopy Reviews v. 40, p. 103–145 (2005)

Probing charge extraction and recombination in fullerene and non-fullerene photovoltaic by transient optical and electrical measurements

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Organic photovoltaics (OPV) are a pivotal technology for transition towards renewable energy. The remarkable progress in power conversion efficiency (PCE) in the last decades is mainly attributed to the evolution from fullerene-based molecular acceptors (PCE ~ 3-4%) to non-fullerene systems (PCE over 20%) [1,2]. Understanding the kinetic competition between charge extraction and recombination is critical to further optimizing these devices. In this work, we employ Transient Photocurrent (TPC) and Transient Photovoltage (TPV) measurements simultaneously with Transient Absorption (TA) spectroscopy. TPC offers insights on charge extraction dynamics, while TPV probes the charge recombination dynamics. This approach allows for a direct correlation between the photogenerated carrier population measured by TA and the resulting electrical signals under identical measurement conditions. We have investigated a systematic range of active layers, from the initial fullerene-based blends P3HT:PC61BM and PTB7-Th:PC71BM, to those containing non-fullerene acceptors (NFA) such as PBDB-T:IDIC and the state-of-the-art PM6:Y6. By comparing TA and TPC dynamics in the short-circuit regime, we directly probe the charge extraction dynamics and try to quantify charge recombination losses. Our results reveal that NFA blends exhibit significantly faster extraction lifetimes, which correlates well to their higher charge carrier mobilities. Furthermore, fullerene materials exhibit a long TA decay well beyond the majority of charge extraction (TPC), a signature of high charge trapping and recombination losses that limit the fill factor and device performance [3]. This work demonstrates that simultaneous TA and TPC/TPV measurements are a robust methodology to probe charge dynamics in OPV, and shows that suppressing charge losses remains one of the primary frontiers for the next generation of OPV materials engineering.

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References

[1] C. Chen et al., Nat. Commun. 15, 1381 (2024).

[2] H. Chen et al., Nat. Mater. 24, 444 (2025).

[3] D. R. B. Amorim et al., Phys. Rev. Appl. 14, 034046 (2020).

Scalability of water-based nanoparticles for active layers in organic photovoltaics

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Organic photovoltaics (OPVs) are generally made of active layers composed of semiconductive polymers and molecules thin films, obtained by printing inks from organic solvents such as chloroform and chlorobenzene, offering advantages such as flexibility and transparency. The change of chlorinated solvent is an important characteristic of sustainability that can be achieved when the active materials are restricted to nanoparticles and form a stable suspension in water. However, the scalability of these polymer nanoparticle solutions remains a major challenge because their properties are difficult to predict. In this context, the aim of this study was to investigate whether operational parameters optimized for a duplicated recipe of the donor polymer P3HT could be applied to triplicated formulations and to donor:acceptor materials inside the same structure. The polymer P3HT was chosen due to the extensive literature on this material, although the final objective of this work is to widen the experiments to other materials currently used in the area. All the aqueous inks were successfully produced via miniemulsion, while adjusting ultrasonication conditions and component proportions. The film depositions were made to analyze the nanoparticles formed by doctor blade, spin coating and drop casting. The morphological analysis by scanning electron microscopy showed that the films were homogeneous and the nanoparticles of donor polymer as well as donor:acceptor presented a spherical shape. Additionally, the optical characterization by ultraviolet-visible absorption spectra confirmed, by the characteristic curve of each component, successful nanoparticle formation. Finally, the conductivity was obtained by current-voltage analysis, to determine the practical feasibility of using those inks as active layers in OPVs. The results show that scalable production of high-quality aqueous nanoparticle inks can be achieved through changes in specific parameters during production.

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References

MAJEWSKI, J. K. Nanoarquitetura de semicondutores orgânicos à base de água para aplicação em camadas ativas de células solares. 2025. 183 f. Dissertação (Mestrado em Física) - Setor de Ciências Exatas, Universidade Federal do Paraná, Curitiba, 2025. Disponível em: https://hdl.handle.net/1884/96346.

BASSI, M. de J. Propriedades optoeletrônicas de materiais orgânicos aplicadas em célula solar e biossensor. 2021. 134 f. Tese (Doutorado em Física) - Setor de Ciências Exatas,

Universidade Federal do Paraná, Curitiba, 2021. Disponível em: https://hdl.handle.net/1884/71616.

Screen-Gate Based Organic Transistors for Adaptive Sigmoid and Gaussian Activation Functions

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Tunable analog activation functions are essential for energy-efficient artificial intelligence (AI) hardware. We present two transistor designs: the sigmoid-like activation function transistor (SA-transistor) and the Gaussian-like activation function transistor (GA-transistor), which implement analog sigmoid and Gaussian functions using a screen gate structure. In the SA-transistor, adjusting the screen gate voltage (VScreen-G) enables precise control of the sigmoid slope and saturation level. In the GA-transistor, the amplitude and standard deviation of the Gaussian response are tunable through the same mechanism. These transistors enable precise and continuous tuning of analog activation parameters such as slope, amplitude, and width at the device level. This controllability allows hardware-optimized neural computations tailored to specific tasks or datasets. Applied in real-world tasks, the SA-transistor improved lung magnetic resonance imaging (MRI) classification accuracy from 77% to 84%, and the GA-transistor raised time-series forecasting coefficient of determination (R2) from 0.82 to 0.93. Furthermore, by assembling these devices into a hardware-based multilayer perceptron (MLP), we demonstrated robust inference on the IRIS dataset with 96.7% overall accuracy. This system-level validation highlights that analog activation transistors can directly support neuromorphic accelerators without digital post-processing, reducing circuit complexity and power consumption while maintaining high classification fidelity.

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References
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Solid Dopant Matrices Based on Microfibrillated Cellulose and KCl for High Performance Organic Transistors

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Electrolyte-Gated Transistors (EGTs) are pivotal for bioelectronics due to their low-voltage operation and high capacitance at the electrolyte/semiconductor interface. However, liquid electrolyte leakage and the need for complex reservoir structures hinder scalability. Microfibrillated cellulose (MFC) emerges as a sustainable alternative due to its high surface area, porosity, and hygroscopic nature. In this study, we explore MFC as an active solid-dopant matrix (SDM) that modulates ion delivery and stabilizes the organic EGTs. Gold electrodes were deposited on glass substrates, followed by the spin-coating of the organic semiconductor P3HT. The SDM was prepared by dispersing MFC in deionized water, followed by the incorporation of KCl (0.1 M) (MFC:KCl). Four configurations were tested: (i) H2O; (ii) MFC:H2O; (iii) KCl:H2O; and (iv) MFC:KCl:H2O. Electrical characterization was performed to obtain transfer and output curves. The pure MFC matrix demonstrated water retention, providing an Ion/Ioff ratio of 102, equivalent to reference liquid-gate devices. The MFC:KCl resulted in a dual-functional effect. First, it provided a stable ion supply for the formation of the Electrical Double Layer (EDL). Second, it compressed the operational electrochemical window. While KCl:H2O electrolytes showed instability at high gate bias, the MFC:KCl-based EGTs remained stable up to VG = -2 V. This stability is attributed to the structure of the cellulose fibers, which limits the mobility of larger solvated ions and prevents premature degradation of the semiconductor/electrolyte interface. The maximum transconductance reached 3×102 mS, with drain currents in the 10-3 A range. We demonstrated an efficient EGT architecture based on an MFC:KCl solid dopant matrix, showing that the cellulose framework enables both field effect and electrochemical modulation while supporting a simplified approach aligned with sustainable, high performance flexible electronics.

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References

Fortunato, E.; Correia, N.; Barquinha, P.; Pereira, L.; Gonçalves, G.; Martins, R. IEEE Electron Device Letters, 29, 9 (2008)

Thiemann, S.; Sachnov, S. J.; Pettersson, F.; Bollström, R.; Österbacka, R.; Wasserscheid, P.; Zaumseil, J. Adv. Funct. Mater. 24 (5), 625 (2014)

Dai, S.; Chu, Y.; Liu, D.; Cao, F.; Wu, X.; Zhou, J.; Zhou, B.; Chen, Y.; Huang, J. Nat. Commun. 9 (1), 1 (2018)

Surface Thermodynamics, Wettability, and Optoelectronic Properties of Anodized Al_2O_3 Films Under Programmable Voltage Control

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Thin anodized aluminum oxide (Al_2O_3) films [1] have attracted significant interest due to their high chemical stability, dielectric properties, and tunable surface morphology, making them promising materials for interfacial engineering in electronic applications. This material also presents high electrical resistivity, optical transparency over a wide spectral range. These properties make anodized oxides particularly relevant for electronic devices such as memories [2] and transistors, where the oxide layer often directly influences device performance. In this work, we investigate the influence of electrochemical anodization parameters on the electrical resistivity, optical properties, wettability, and surface thermodynamics of Al_2O_3 films. The oxide layers were fabricated using a programmable anodization system controlled by a graphical user interface developed within the research group. This software-based platform allows precise control of key experimental parameters, including applied voltage, anodization time, and voltage ramp profiles, enabling systematic and reproducible modulation of oxide growth conditions. Surface wettability was evaluated by static contact angle measurements, providing quantitative information about interfacial behavior. The wetting response was analyzed using thermodynamic models, particularly the Cassie–Baxter [3]. The correlation between anodization parameters and contact angle values revealed systematic trends in the formation of different surface topographies and energetic states. UV–Vis measurements showed that growth parameters such as anodization time and applied voltage significantly affect optical transmittance, leading to increased transparency as the oxide layer develops. Overall, the results demonstrate that programmable anodization provides an effective strategy for tuning the interfacial energetics and functional properties of Al_2O_3 films.

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References

[1] J. W. Diggle, Thomas C. Downie, and C. W. Goulding, "Anodic oxide films on aluminum”, chemical Reviews Vol 69 nº3, pp 365-405, jun. 1969DOI: 10.1021/cr60259a005

[2] G. S. M. de Araújo et al., “ITO/polymer/Al from diode-like to memory device: electroforming, multilevel resistive switching, and quantum point contact,” Journal of Materials Science: Materials in Electronics, vol. 35, no. 3, Jan. 2024, doi: 10.1007/s10854-024-11952.

[3] A. J. B. Milne, A. Amirfazli, “The Cassie Equation: How it is meant to be used”. Advances in Colloid and Interface Science, vol.170, pp. 48–55, 2011, doi: 10.1016/j.cis.2011.12.001.

Thermal Cycling-Driven Degradation of Perovskite Solar Cells by In Operando nano-XRD

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Metal halide perovskites (MHPs) have emerged as promising photovoltaic materials due to their elevated charge carrier mobility, high power conversion efficiency (PCE), and low exciton binding energy [1,2]. Perovskite solar cells (PSCs) have already demonstrated PCE values exceeding 26% [3]. However, despite rapid efficiency improvements, long-term operational stability and a fundamental understanding of degradation mechanisms at the nanoscale remain limited. Previous studies indicate that day–night illumination cycles accelerate PSC degradation [4], alongside effects such as thermally induced surface restructuring [5], light-induced phase segregation, and interfacial iodine migration under illumination [6]. Nevertheless, nanoscale and in operando investigations to explain these mechanisms are still lacking. To address these challenges, we investigate the structural heterogeneities of a conventional n–i–p $Cs_{0.05}FA_{0.95}PbI_3$ solar cell under thermal cycling using advanced synchrotron-based characterization techniques. By mapping the evolution of bulk d-spacing, we provide insights into the fundamental processes governing PSC instability and contributing to the advancement of their large-scale commercialization.

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References
Raphael, E et al., Quim. Nova 41, 61 (2018).

Kimberley J. Savill, Aleksander M. Ulatowski, and Laura M. Herz ACS Energy Lett. 6, 2413-2426 (2021)

Li, Bin et al. Adv. Mater., e23630 (2026).

Tuning the Operating Mode of P3HT Electrolyte-Gated Transistors by Controlling Extra Ions Mixed into a Honey-Based Electrolyte

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Electrolyte-gated transistors (EGTs) capable of operating as either Electrolyte-Gated Field-Effect Transistors (EGFETs) or Organic Electrochemical Transistors (OECTs) are highly desirable for their flexibility in applications such as sensing and neuromorphic computing. The most common strategy to achieve these different modes is to explore various semiconductor materials [1]. In contrast, this work focuses on engineering the electrolyte. We demonstrate that by formulating different electrolytes based on honey, a natural and eco-friendly resource, we can effectively tune the operating mode of P3HT-based EGTs. The proposed device architecture consists and explore just one semiconductor that is the poly(3-hexylthiophene-2,5-diyl) (P3HT) as channel, and a commum based-electrolyte layer based on honey that was used pristine and added by different ions producing also, honey mixed with lithium perchlorate ($LiClO_4$) and honey mixed with the ionic liquid 1-Ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide ([EMIM][TFSI]). The incorporation of additional ionic species into the electrolyte induced a shift in the transistor's operational mode, transitioning it from an EGFET (with pristine honey) to an OECT. When evaluated as sensors, traditional figures of merit such as threshold voltage and transconductance revealed clear distinctions in the signal response of the different EGTs. When analyzed as a neuromorphic transistor, it enabled the generation of different types of artificial synapses, operating through mechanisms such as electrical double layer formation and ionic doping. The exploration of different electrolyte compositions leads to variations in operating mode, response times, and emulation intensity, including paired-pulse facilitation (PPF). The results obtained in this work show honey as a versatile electrolyte to be explored in sensing and neuromorphic devices, seen as a possible alternative to the use of water as a universal electrolyte in EGTs.

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References

G. Schweicher, G. Garbay, R. Jouclas, F. Vibert, F. Devaux, and Y. H. Geerts, Molecular semiconductors for logic operations: Dead-end or bright future?, Advanced Materials 32, 1905909 (2020).

Urbach Energy in MEH-PPV

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Understanding how structural order, aggregation, and vibrational coupling influence the optical and electronic properties of conjugated polymers is essential for optimizing their performance in optoelectronic devices. Here, we compare MEH-PPV films prepared by the Langmuir–Blodgett (LB) technique with disordered drop-cast films and with the polymer in solution. UV–Vis absorption, steady-state photoluminescence, polarized spectroscopy, Raman scattering, and charge-transport measurements were employed. In solution, variations of the optical gap and the Urbach tail with concentration reveal early aggregation effects, manifested in the absorption tail before significant perturbation of the conjugated backbone. LB films exhibit partial orientational order, evidenced by absorption dichroism and polarized emission, whereas drop-cast films show similar optical responses along perpendicular directions. Despite this orientational order, the Urbach energy in LB films remains similar parallel and perpendicular to the dipping direction, indicating that the distribution of optical defects is not direction-dependent. However, its thickness dependence highlights the role of interface effects. Vibronic analysis (Huang–Rhys factor and effective conjugation length) shows that LB deposition preferentially aligns polymer segments with longer conjugation lengths and modifies the vibrational modes coupled to emission, consistent with Raman measurements. Electrical current density versus electric field measurements further distinguishes the morphologies: LB devices exhibit smoother transitions between ohmic and space-charge-limited current (SCLC), whereas drop-cast devices reach the trap-filled limit regime at lower fields, indicating lower trap density distributed over a broader energy range. The comparison between optical (Urbach) and electrical (TFLC) analyses confirms that shallow optical traps and deep electrical traps probe distinct disorder populations.

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314034/2023–4.

References

Ugur, E.; Ledinský, M.; Allen, T. G.; Holovský, J.; Vlk, A.; De Wolf, S. Life on the Urbach Edge. Journal of Physical Chemistry Letters. American Chemical Society August 25, 2022, pp 7702–7711. https://doi.org/10.1021/acs.jpclett.2c01812.

Zarrabi, N.; Sandberg, O. J.; Meredith, P.; Armin, A. Subgap Absorption in Organic Semiconductors. Journal of Physical Chemistry Letters. American Chemical Society April 6, 2023, pp 3174–3185. https://doi.org/10.1021/acs.jpclett.3c00021.

Urban deployment and performance analysis of organic photovoltaic devices: Experimental and theoretical insights

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Organic photovoltaic (OPV) technologies have attracted considerable interest as sustainable alternatives to conventional silicon-based solar cells due to their flexibility, lightweight nature, and semi-transparency, which make them particularly suitable for building-integrated photovoltaic applications. In this study, the real-world performance and degradation mechanisms of commercial OPV modules produced by SUNEW (Brazil) were investigated through a 22-month outdoor monitoring campaign at the Federal University of Paraná (UFPR), where the modules were installed on glass facades and rooftops. Electrical characterization was performed according to ISOS protocols under illuminated (O-2) and dark (D-1) conditions. Using the J-V characteristics in dark, charge transport mechanisms were evaluated using thermionic emission and space-charge-limited current (SCLC) models. The results revealed a progressive increase in series resistance and a transition from injection-limited to transport-limited conduction, indicating degradation-induced limitations in charge transport. Complementary Atomic Force Microscopy (AFM) and X-ray Photoelectron Spectroscopy (XPS) analyses evidenced morphological, compositional, and chemical modifications in the polymeric layers after prolonged environmental exposure, particularly involving oxygen- and sulfur-containing species. The combined electrical and surface analyses provide insights into the operational stability of OPV panels under tropical climatic conditions and highlight key degradation pathways that affect charge mobility and overall device performance. The results contribute to understanding OPV lifecycle behavior and to improving the design and durability of next-generation organic solar technologies.

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References
Santos, T. R. C., Koeb, G. M., Pacheco, K. R. M., das Neves, M. F. F., Benatto, L., Veiga, A.

G., … & Roman, L. S. (2026). Urban deployment and performance analysis of organic photovoltaic devices: Experimental and theoretical insights. Solar Energy Materials and Solar Cells, 304, 114426.

Water-based nanoparticle-printed thin films for scalable and sustainable organic photovoltaic devices

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Water-processable organic semiconductors represent a promising route toward sustainable synthetic electronic materials while preserving control over molecular organization and optoelectronic properties. Here, we investigate semicrystalline donor, acceptor, and donor–acceptor nanoparticles prepared via miniemulsion and processed as aqueous inks for slot-die coating. This strategy enables homogeneous thin-film deposition and promotes controlled self-assembly during film formation. Optical and structural characterization reveals enhanced intermolecular ordering in nanoparticle-derived films compared to chloroform-processed references. UV–vis absorption and photoluminescence spectra display redshifted transitions and more resolved vibronic features, indicating extended effective conjugation length. Scanning electron microscopy confirms uniform and compact morphologies. Spectroscopic ellipsometry provides detailed analysis of the complex refractive index, evidencing increased molecular packing density and preferential edge-on orientation, structural features that are directly linked to improved charge-transport pathways in conjugated systems. Photovoltaic devices fabricated from these water-based nanoparticle films exhibit promising performance, demonstrating that environmentally benign processing can simultaneously enhance semicrystalline organization and functional properties. These results demonstrate that nanoparticle-based aqueous processing provides a consistent route to modulate molecular organization in conjugated thin films. The approach offers a robust framework for systematically investigating structure–property relationships in emerging organic semiconductors and for extending this strategy to additional material systems.

References

M. de Jesus Bassi, J. K. Majewski, and L. S. Roman, in Contribution of Colloidal Materials to Air, Water and Soil Environmental Sustainability From Basic Concepts to Advanced Applications, ed. I. C. Riegel-Vidotti, L. M. Zimmermann, and H. R. de Barros, Royal Society of Chemistry, 2025, ch. 7, pp. 125-151.

Cool plastics for a greener world

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Keywords: Optoelectronic devices, light and heat management, photonic structures

With seabirds trapped in multipack drink rings, and mid-ocean islands of indestructible rubbish, the idea that plastics could play a big part in a sustainable future world might seem far-fetched. However, new smart plastics may yet rescue the reputation of this all-consuming 20th century material. Research into ‘cool plastics’ for cars and buildings could reduce the need for air conditioning and, thus, improve their energy efficiency. We will present recent efforts to design plastics of desired optical functions targeted for a greener world. We will discuss the potential of such systems that can offer the same flexibility, softness and light weight as commodity plastics but can control the flow of light and heat therefore assisting energy management in buildings and greenhouses in the form of heat mirrors, photovoltaic applications when used as anti-reflection coatings and semi-transparent mirrors, as well as building blocks for novel optical structures that can lead to quantum devices.

The rise of organic and inorganic two-dimensional materials for interface engineering in perovskite photovoltaics

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Keywords: Halide Perovskite, Two-dimensional materials, Solar Cells, Photovoltaics

The performance and long-term durability of perovskite solar cells and modules are strongly governed by the chemical and electronic properties of buried and top interfaces. In this talk, we present a unified overview of interface engineering strategies based on inorganic and organic two-dimensional interlayers for perovskite photovoltaics.
Inorganic 2D interlayers [1-3] offer a direct route to tune the electronic landscape of the device. In particular, MXenes enable work-function modulation of both the perovskite absorber and charge-transport layers, while also inducing interfacial dipoles that reshape band alignment and facilitate charge extraction. Ultraviolet photoemission spectroscopy and density functional theory, as reported in the earlier work, showed that these 2D carbides can tailor interface energetics without detrimental alteration of the bulk electronic properties, resulting in reduced hysteresis and substantial performance gains. This concept was later extended to advanced architectures, where MXene in combination with organic functional molecules-enabled interfacial design contributed to the formation of nanoscale field-effect junctions in semitransparent perovskite top modules for four-terminal perovskite/silicon tandems, highlighting the broader utility of inorganic 2D materials in scalable photovoltaics.
Organic and hybrid 2D interlayers [4-5] complement this approach by providing strong chemical passivation and improved structural stability at the perovskite surface. In the uploaded studies, bulky organic cations were used to form 3D–2D junctions in wide-bandgap semitransparent perovskite solar cells, enabling improved interfacial quality, higher open-circuit voltage, and enhanced light utilization efficiency in large-area transparent devices and modules. More recently, co-crystal engineering of a two-dimensional perovskite phase using a neutral molecular linker was shown to overcome some of the intrinsic stability limitations of conventional ionic 2D interlayers, delivering high efficiencies together with remarkable resistance to light soaking, ultraviolet exposure, and thermal stress in both small-area devices and large-area modules.

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References:

[1] A. Agresti, A. Pazniak, S. Pescetelli, et al. Nature Materials 18, 1228–1234 (2019).
[2] S. Pescetelli, A. Agresti, G. Viskadouros. et al. Nature Energy 7, 597–607 (2022).
[3] A. Agresti, S. Pescetelli, et al. Nature Communications 17, 3394 (2026)
[4] N. Yaghoobi Nia, M. Zendehdel et al. Nature Energy 11, 135–149 (2026)
[5] D. Di Girolamo, F. Matteocci et al. Advanced Energy Materials 14, 2400663 (2024)

Chiral Optoelectronics for Next-Generation Displays and Photodetectors

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Keywords: chiral optoelectronics, chiral organic semiconductors, chiral perovskites, circularly polarized light, photon spin.

The precise control of photon spin states, known as circular polarization (CP), is emerging as a cornerstone for the next generation optoelectronics. Chiral organic materials and chiral perovskites have garnered significant attention due to their unique ability to directly emit or detect circularly polarized light (CPL) without the need for bulky external filters. I will present synthesis of chiral organic semiconductors, fabrication of supramolecular semiconducting materials, structure-property relationships, and their applications in advanced optoelectronic sensors and CPL emitters. In addition, a simple yet powerful method to fabricate chiroptical flexible layers via supramolecular helical ordering of conjugated polymer chains will be introduced. These findings provide guidelines for enhancing chiroptical properties using multiscale chirality and rational molecular design of organic semiconductors toward high-performance chiral optoelectronics. In addition, methodologies for boosting chiroptical activities of chiral perovskites will also be presented. These results demonstrate an effective strategy to realize on-chip detection of the spin degree of freedom of photons necessary for encoded quantum information processing and high-resolution polarization imaging, in addition to high-efficiency 3D displays.

Chiroptical switching and logic operations using photoexcited states

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Keywords: Molecular photonics, chiral materials, circular dichroism, spectroelectrochemistry, organic semiconductors, radical anions.

Chiroptical switches are made of chiral materials that can be reversibly switched between two (or more) states with distinctively different chiroptical signals. These materials hold great promise in applications such as chiral sensing, nonlinear optics, molecular-level optoelectronic devices and catalysis. [1] Here, I will describe the design and functionality of redox-modulated molecular switching in the ground and excited states.

In the ground state, binaphthyl-based chiral materials demonstrate fatigue-resistant, reversible redox-controlled optical switching. We use various spectroelectrochemical (SEC) techniques to characterize the reduced states of binaphthyl materials in situ, a method that remains one of the few examples in the literature. [2-3] In excited states, these binaphthyl materials can undergo energy and electron transfer, resulting in triplet and ionic states, respectively. By employing unpolarized and circularly polarised pump-probe transient absorption spectroscopy under applied electric fields, we identify distinct optical signatures of triplet states and anions that are observable across a range of electric field strengths. We utilize these properties to demonstrate AND and INH (inhibit) logic operations with these excited states and propose extending this approach to more complex circuits, such as a Half Adder. This work provides a framework for combining light and electric fields/applied potentials to create exciton circuitry.

References:

[1] LA Hall, et al., *Chem Soc Rev*, **52**, 3567 (2023).
[2] LA Hall, et al., *J. Phys. Chem. Lett.*, **16**, 1529 (2025).
[3] LA Hall, et al., *Chem. Mater.*, **38**, 705 (2026).

Connecting Mechanical Properties, Durability, and Reliability of Perovskite Solar Cells

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Keywords: perovskite solar cells, flexible, rigid, mechanical behavior, durability, reliability

The unproven durability of perovskite solar cells (PSCs) is likely to pose significant technical hurdles in the path towards the widespread deployment of this burgeoning thin-film photovoltaics (PV) technology. The overall durability and reliability of rigid and flexible perovskite solar cells, which is related to the operational-stability, is directly affected by the mechanical properties of metal-halide perovskite thin films, other layers, and interfaces, but this connection has been largely overlooked. This is particularly important in flexible PSCs on polymer substrates, which are subjected to much higher mechanical stresses. Thus, there is a sense of urgency for addressing the mechanical reliability issue comprehensively, and help PSCs reach their full potential. To address these final technical hurdles, several rationally-designed interfacial tailoring approaches are used to enhance the mechanical properties of both rigid PSCs and flexible PSCs. Most importantly, these approaches are designed such that they also increase efficiency of PSCs. The important challenges and opportunities, together with best practices, pertaining to the three key interrelated elements that determine the mechanical reliability of PSCs are discussed: (i) driving stresses, (ii) mechanical properties, and (iii) mechanical failure. The scientific rationales for these approaches to improve the mechanical properties are also discussed, together with the presentation of examples where failure-mitigation results in more efficient, durable, and reliable PSCs.

Contact Modulation in Perovskite/Organic Optoelectronic Device

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Abstract

The interface contact in perovskite and organic solar cells is a critical factor that significantly influences both the performance and stability of these devices. It serves as a conduit for charge transfer between different layers, which is essential for minimizing recombination losses and thereby enhancing the overall efficiency of the solar cells. A well-engineered interface ensures that there is optimal energy level alignment, which is crucial for improving charge extraction and transport across the device. This not only boosts efficiency but also contributes to the operational stability of the solar cells. Moreover, the interface plays a vital role in the longevity of the device by preventing various degradation pathways that can occur over time. Degradation can severely impact the performance and lifespan of solar cells, so a robust interface is key to maintaining long-term functionality. Therefore, a deep understanding of these interfaces and their optimization is essential for advancing solar cell technology and achieving higher power conversion efficiencies. In this talk, we will focus on discussing various contact modulation strategies employed in perovskite solar cells, organic solar cells, and their tandem applications. These strategies are designed to enhance interface properties, thereby improving device performance and stability. By exploring these approaches, we aim to shed light on the latest advancements and future directions in solar cell technology.

References

[1]. “Inorganic perovskite/organic tandem solar cells with 25.1% certified efficiency via bottom contact modulation”, Nature Energy, 10,513-525, 2025
[2]. “Perovskite-Organic Tandem Solar Cells with Superior Reverse Bias Stability”, Nature Materials, 10.1038/s41563-026-02541-6, 2026

Design and Synthesis of Functional Organic Materials for Hybrid Photonic Devices

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Keywords: Functional Organic Materials, Perovskite Solar Cells, Bio-Light-Emitting Devices

The rational molecular design of π-conjugated organic materials is a keystone in the development of next-generation optoelectronic and hybrid photonic devices.
Organic hole transport materials (HTMs) are crucial components in perovskite solar cells (PSCs), enabling efficient hole extraction and suppressing interfacial recombination.
In parallel, functional organic materials are gaining increasing attention for bio-integrated light-emitting devices (Bio-LEDs). These systems require molecularly engineered emitters combining high photoluminescence efficiency, and compatibility with biological environments.
At the Functional Organic Materials Group of the University of Turin, our research focuses on the design, synthesis, and characterization of novel organic functional materials for optoelectronic applications. We develop advanced, low-cost and semi-transparent hole transport materials (HTMs) for perovskite solar cells[1,2], with particular interest in devices engineered for space applications, where lightweight architectures, high specific power, and radiation tolerance are critical requirements. In parallel, we design tailored organic emitters for Bio-LEDs[3], establishing clear correlations between molecular structure, and optoelectronic performance. By integrating synthetic organic chemistry, electrochemical and spectroscopic characterization, and device-level evaluation, we aim to contribute to the development of sustainable organic and hybrid photonic technologies.

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References:
[1] V. Maruzzo, et al., *Sol. Energy Mater. Sol. Cells.*, **290**, 113697, (2025)
[2] D.A. Machado de Alencar, et al., *Adv. Sustainable Syst.*, **9**, 2400674 (2025).
[3] S. Ferrara, et al., *Adv. Funct. Mater.*, **32**, 2111381 (2022).

From Displays to Data Links: High-Speed Organic Optoelectronics for Visible Light Communication

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Abstract

We report recent advances in the development of organic optoelectronic devices for visible light communication. Our work expands the range of applications of organic semiconductors and shows that they can be much faster than previously thought. We show that by addressing limiting processes of electrical time constant and charge transit time we can make exceptionally fast organic light-emitting diodes and photodiodes for optical communication. We demonstrate record communication rates for organic devices of 4 Gbps for a single organic light-emitting diode, and 3 Gbps for a single photodiode. Our results show that OLEDs can be used to make fast transmitters for communication-enabled displays and lighting systems, and that organic photodiodes can be used as receivers.

Hybrid Perovskite Photodetectors

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Keywords: Photodetectors, Perovskites

Perovskite, a flexible and versatile semiconductor material, exhibits remarkable optoelectronic properties, including a high light absorption coefficient, micrometer-scale carrier diffusion length, high mobility, and exceptional defect tolerance. These outstanding semiconductor characteristics have expanded the potential of perovskite materials beyond traditional photovoltaic applications.
My research group has been focused on advancing the preparation of materials, exploring physical properties, optimizing device structures, and integrating functional systems for various light-sensing applications.
In this report, I will present our progress in developing high-performance perovskite thin films for photodetectors with enhanced detectivity and rapid response times. These photodetectors serve as essential components for applications such as micro-spectrometers, multimodal hyperspectral imaging, and anti-noise, spatially coupled optical communication systems.

Acknowledgements: National Natural Science Foundation of China

References:
[1] Liang Li, et al, *Nat. Mater.*, **24**, 1778, (2026)
[2] Liang Li, et al, *Adv. Mater.*, **34**, 2200221, (2022)
[3] Liang Li, et al, *Adv. Mater.*, **36**, 2402253, (2024)
[4] Liang Li, et al, *Adv. Mater.*, **36**, 2400279, (2024)
[5] Liang Li, et al, *Nat. Commun.*, **15**, 2066, (2024)

Integrated Energy Harvesting and Storage for Autonomous Sensor Networks

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Keywords: photocapacitors, coordination polymers, IoT, ambient energy, edge computing, sustainability

Abstract

Copper coordination compounds from extended polymers to discrete redox shuttles provide earth-abundant, solution-processable building blocks for every layer of an autonomous indoor energy system. Photocapacitors that monolithically integrate photovoltaic harvesting with supercapacitive storage on a single substrate are emerging as a key architecture for battery-free IoT, yet their performance has been limited by inefficient charge-selective contacts and narrow spectral harvesting [3]. This talk traces how copper coordination chemistry addresses these bottlenecks from the molecular to the system level. First, mixed-valence Cu(II)/Cu(I) dithiocarbamate–halide coordination polymers are introduced as dopant-free hole conductors. Switching the bridging halide from bromide to iodide enhances Cu–I valence-band conjugation, reducing the computed effective hole mass from $94m_e$ to $6m_e$ and raising conductivity over two orders of magnitude to 1 mS cm^{-1}. In carbon-electrode perovskite solar cells the iodide polymer reaches 13.8% PCE nearly double that of doped Spiro-MeOTAD and retains >94% efficiency over 50 days under ambient humidity [1]. Second, we leverage discrete $Cu(tmby)_2$ redox shuttles in dye-sensitized solar cells (DSCs) that exceed 30% PCE under 1000 lux and couple them with polyviologen/carbon asymmetric supercapacitors on a shared PEDOT electrode to form three-terminal photocapacitors. Under ambient light these devices deliver 920 mV and 18% overall charging efficiency, sustaining a three-layer edge-AI network for 72 hours outperforming commercial a-Si modules 3.5-fold in inference throughput and reaching 93% CIFAR-10 accuracy at 0.81 mJ per classification [2]. These results demonstrate how tuneable redox potentials and solution processability in copper coordination compounds propagate from molecular design through device integration to system-level energy autonomy for battery-free computing.

[1] H. Michaels, M.J. Golomb, B.J. Kim, T. Edvinsson, F. Cucinotta, P.G. Waddell, M.R. Probert, S.J. Konezny, G. Boschloo, A. Walsh, M. Freitag, J. Mater. Chem. A, 10, 9582 (2022)

[2] N. Flores-Diaz, F. De Rossi, T. Keller, H. Morritt, Z. Perez Bassart, A. Lopez-Rubio, M.J. Fabra, R. Freitag, A. Gagliardi, F. Fasulo, A.B. Muñoz-García, M. Pavone, H.J. Lomeri, S. Sanchez Alonso, M. Grätzel, F. Brunetti, M. Freitag, Energy Environ. Sci., 18, 4704 (2025)

[3] N. Flores-Diaz, F. De Rossi, A. Das, M. Deepa, F. Brunetti, M. Freitag, Chem. Rev., 123, 9327 (2023)

Interface engineering for improved efficiency and lifetime in organic solar-cells

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Understanding and minimizing non-radiative recombination pathways has been instrumental in increasing the power-conversion efficiencies (PCE) in organic photovoltaics (OPV) to well above 20%, almost doubling the PCE in the past five years. However, given the fast development of the efficiencies, the stability of these solar cells still needs improvement.

Inverted organic solar cells are attractive alternatives for increasing lifetimes, due to the advantage that a high-work-function top electrode can be used. Non-radiative recombination in any form, i.e. trap-assisted, or surface recombination of minority carriers at the (wrong) electrode will inevitably lead to lower efficiencies

In this talk, we will focus on the passivation of metal-oxides in inverted OPVs. We will show that (weak to moderate) doping caused by metal evaporation and/or interaction between charge transport layers and the photoactive layer is a common cause for increased losses.[1,2] We will also show how these factors can be mitigated with increased efficiency and lifetime as a result.

[1] Liu, B.; Sandberg, O. J.; Qin, J.; Liu, Y.; Wilken, S.; Wu, N.; Yu, X.; Fang, J.; Li, Z.; Huang, R.; Zha, W.; Luo, Q.; Tan, H.; Österbacka, R.; Ma, C.-Q. *Nat. Photonics* **2025**, *19* (2), 195–203..

[2] Xi, Q.; Qin, J.; Sandberg, O. J.; Wu, N.; Huang, R.; Li, Y.; Saladina, M.; Deibel, C.; Österbacka, R.; Ma, C.-Q. *ACS Appl. Mater. Interfaces* **2025**, *17* (10), 15456–15467.

Narrow OLED Emitters by Multiresonant Dyes based on Aromatic/Antiaromatic and Quinoidal Designs

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Keywords: narrow emitters, photoluminescence, organic molecules, multiresonant dyes

Multiresonant organic molecules and dyes are of present interest in several molecular designs for organic photonics.[1] In particular, these molecules have been targeted as thermally activated delayed fluorescence, in narrow emitter designs, in organic molecules with inverted singlet triplet gap, etc.[2] The most popular design of multiresonant organic materials is based on crossed functionalization of aromatic benzene dyes based with electron donor para-(amino, amino) groups and electron acceptor para-(boron, boron) moieties.[1] The atomic segmentation of the wavefunctions of the frontier orbitals is the key aspect in these strategies. Here, we present new chemical designs for multiresonant organic molecules with para-bis(amino) groups and quinoidal spacers (**2** in Figure 1) with mixture of aromatic and antiaromatic groups[3] (i.e., pure hydrocarbon, **3** in Figure 1). A complete photophysical study accompanied with OLED features and quantum chemical calculations will be presented. In addition, the application of these dyes as amplification of light emission and laser devices applications will be discussed.

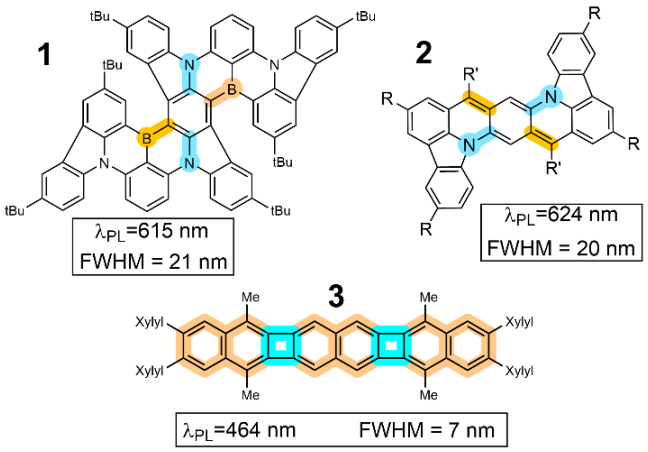


Figure 1: Chemical structures of the reference molecule in the field (**1**) and of two examples of the azaquinoidal design (**2**) and of the aromatic/antiaromatic design (**3**).

Acknowledgements: The Spanish Ministry of Science and Innovation is acknowledged for the project reference PID-2024- 157601NB-I00.

References:

[1] T. Hatakeyama, *Advanced Materials*, **28**, 2777, (2016).
[2] C. Adachi, T.Hatakeyama, *J. Am. Chem. Soc.*, **145**, 1505, (2023).
[3] Y. Xia, *J. Am. Chem. Soc.*, **139**, 15933, (2017).

Organic semiconductors as a platform for molecular photonics: from polariton devices to fluid light and neural interfaces

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Keywords: Exciton-polaritons, Biophotonics, Electrochemiluminescence

Organic pi-conjugated materials are uniquely versatile photonic building blocks. Their high oscillator strengths, broad spectral tunability, and compatibility with a wide range of substrates and fabrication methods make them attractive not only for conventional optoelectronics but also for a new generation of devices that exploit the interaction of organic emitters with photonic resonators, electrochemical driving forces, and biological environments. This talk surveys recent advances from our group at the intersection of organic semiconductors, photonics, and the life sciences.

When organic emitters are placed in optical microcavities under strong light-matter coupling conditions, the resulting exciton-polaritons open design space not accessible in conventional thin-film architectures. We have used this to develop polariton OLEDs that combine narrowband, angle-independent emission with EQE exceeding 20%, now demonstrated across the visible and into the NIR. The same physics enables thin-film optical filters with angle-independent pass and stop bands, overcoming a fundamental limitation of conventional interference filters and opening new routes to miniaturised fluorescence sensing. In optically pumped organic lasers, engineering polariton confinement — through morphology control or active-layer micropatterning — has yielded record-low lasing thresholds and a route to metallic-mirror cavities compatible with electrical pumping.

Stepping away from solid-state devices, electrochemiluminescent devices generate light from solutions of pi-conjugated molecules driven electrochemically. We recently introduced electrochemically induced hyperfluorescence via charge-transfer excimers, achieving record luminance and stability in these “fluid light” sources, and demonstrated their use for optogenetic control of neuronal activity.

Finally, miniaturised OLEDs monolithically integrated on CMOS chips provide implantable light sources with single-neuron spatial resolution, enabling precise optical control of neural circuits in living animals — illustrating how organic photonics can reach deep into biology.

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Photo- and Thermal-Stability of Organic Solar Cells

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Organic semiconductor-based solar cells (OSCs) have been considered the most promising solar cell technology for indoor and IoT applications owing to their flexibility, low cost, and potential for large-scale printing. The development of non-fullerene acceptors has enabled the highest power conversion efficiency over 21%. Despite these efficiency gains, the long-term stability of OSCs remains a major challenge before their commercialization.

The SINANO research team in Suzhou has been working on the intrinsic degradation mechanisms of organic solar cells under light, thermal, and electric field stress. In particular, we recently demonstrated that unexpected interfacial degradation at the ZnO and MoO_3 interface is responsible for the photonic and thermal degradation of polymer:non-fullerene solar cells. By proper interfacial protection of ZnO with in situ converted SiOxNy[1] and MoO_3 with low-HOMO fullerene at the anode interfaces,[2-3] the cells showed excellent photo- and thermal stability. Our findings underscore the effectiveness of our approach and provide valuable insights for the design of more stable polymer solar cells.

1. Liu, B.; Sandberg, O. J.; Qin, J.; Liu, Y.; Wilken, S.; Wu, N.; Yu, X.; Fang, J.; Li, Z.; Huang, R.; et al. Inverted organic solar cells with an in situ-derived SiOxNy passivation layer and power conversion efficiency exceeding 18%. *Nat. Photonics* **2025**, 19, 195–203

2. Qin, X.; Yu, X.; Li, Z.; Fang, J.; Yan, L.; Wu, N.; Nyman, M.; Österbacka, R.; Huang, R.; Li, Z.; et al. Thermal-Induced Performance Decay of the State-of-the-Art Polymer: Non-Fullerene Solar Cells and the Method of Suppression. *Molecules* 2023, **28**, 6856.

3. Qin, J.; Xi, Q.; Wu, N.; Liu, B.; Yue, C.; Fang, J.; Wang, Z.; Du, Y.; Zhang, Q.; Wang, Z.; et al. Improved damp heat and thermal cycling stability of organic solar cells. *Nat. Energy* **2025**, 10, 1439–1449

Photokineticism: Comprehensive and quantitative understanding of phenomena from elementary processes

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Keywords: Quantum chemical calculations, Rate constants, OLEDs, TADF, Fermi's golden rule, Photocatalysts

Many phenomena in nature consist of a network of sequential and competing elementary processes. While experiments usually capture the macroscopic outcome, a truly fundamental understanding requires elucidating both all relevant elementary steps and the emergent behavior of the whole system. In photophysical and photochemical phenomena involving emission, not only radiative and nonradiative pathways but also internal conversion, intersystem crossing, reverse intersystem crossing, and excitation energy transfer across multiple electronic states must be evaluated simultaneously and quantitatively, which is far from trivial.

To address this challenge, we have recently developed a rate-constant-based quantum chemical framework that enables comprehensive understanding and quantitative prediction of emission phenomena in organic molecules composed of multiple intertwined processes. With this approach, we have quantitatively predicted the rate constants and quantum yields of all elementary and composite processes, as well as a wide range of time-dependent behaviors, including exciton population dynamics.[1-3]

We are now extending this methodology, which we believe will play a central role in building the fundamental science of exciton dynamics. Inspired by the artistic movement of "*Kineticism,"* where a complex whole is decomposed into rhythmic elements to construct a painting, we have launched a project to establish a new conceptual framework, a theoretical "-ism" of "kinetics" centered on "photo," which we call "*Photokineticism*." In this talk, I will outline this concept and present our recent advances, including those mentioned above.

The method we propose is applicable to a broad spectrum of systems. Recently, we have successfully applied it to photocatalytic systems that suppresses the aggregation of amyloid-β peptides, implicated in Alzheimer's disease and related disorders, while dramatically reducing side effects.[4]

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References:

[1] K. Shizu, H. Kaji, *J. Phys. Chem. A* **125**, 9000 (2021).
[2] K. Shizu, H. Kaji, *Commun. Chem.* **5**, 53 (2022).
[3] K. Shizu, H.; Kaji, *Nat. Commun.* **15**, 4723 (2024).
[4] M. Yamane *et al.*, *J. Am. Chem. Soc.* **147**, 28860 (2025).

Towards scalable fabrication of Sn and Sn/Pb perovskites solar cells

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Keywords: metal halide perovskites, solar cells, Sn-perovskite, Sn-Pb perovskites

The scalable fabrication of perovskite solar cells (PSCs) is a critical challenge in the transition from laboratory-scale research to industrial production. While spin coating has been the dominant method for fabricating the highest efficiency tin-based and Sn-Pb PSCs solar cells, it presents significant limitations in terms of scalability, substrate size, cost, deposition speed, and yield. These constraints hinder the translation of laboratory successes to large-scale manufacturing.

In contrast, blade coating has emerged as one of the most promising techniques for scalable PSC fabrication. Blade coating offers advantages such as high throughput, compatibility with large substrates, and cost-effectiveness**,** making it highly suitable for industrial-scale production. Importantly, the procedures and optimizations developed using blade coating can be readily transferred to industrial-scale techniques, including roll-to-roll and slot-die coating, among others. This transferability is crucial for enabling the mass production of perovskite solar cells with consistent quality and performance.

In my presentation, I will discuss two distinct methods to achieve control over the challenging crystallization of tin-containing perovskite materials. First, I will demonstrate how 3D Sn-Pb perovskites can be obtained by depositing a 2D perovskite and performing a cation exchange [1, 2]. Then, I will present a two-step blade-coating process: the first step involves depositing a non-perovskite precursor, followed by the introduction of organic cations that transform the structure into the desired perovskite composition [3].

After detailing these methods, I will report that solar cell efficiencies exceeding 18% can be achieved using a 50% Pb-Sn composition, while efficiencies above 10% are attainable with a pure Sn composition [4].

References:
[1] J. Xi, H. Duim, M. Pitaro, K. Gahlot, J. Dong, G. Portale, M. A. Loi, Adv. Funct. Mater. **31**, 2105734, (2021).
[2] J. Xi, J. K. Jiang, H. Duim, L. J. Chen, J. X. You, G. Portale, S. Z. Liu, S. X. Tao, M. A. Loi *Adv. Mater.*, **35**, 2302896 (2023).
[3] L. J. Chen, E. K. Tekelenburg, K. Gahlot, M. Pitaro, J. Xi, A. Lasorsa, G. Feraco, L. Protesescu, P. C. A. van der Wel, G. Portale, P. Rudolf, C. J. Brabec, M. A. Loi, Energy Environ. Sci.,**16**, 5315 (2023).
[4] L. Chen, L. Di Mario, G. Portale, C. J Brabec, and M. A. Loi, Adv. Energy Mater., **16**, e03611 (2026).

Abstract: Twisting Light and Spin in Chiral Halide Perovskites

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Chiral hybrid halide perovskites offer a unique platform where structural chirality, lattice dynamics, and spin–orbit coupling converge to generate rich optical and spin-dependent phenomena. Their soft lattices and flexible organic–inorganic frameworks allow strong responses to atomic motion, making them ideal for exploring how lattice dynamics influence light–matter and spin interactions.

Using first-principles and machine-learning–accelerated simulations, we investigate the lattice dynamics, optical activity, and spin textures of two-dimensional chiral lead-halide perovskites. We identify vibrational modes with chiral character, chiral phonons, that couple to excitonic and spin states, modulating both circular dichroism and spin polarization. Temperature-dependent structural fluctuations play a key role in tuning these chiroptical and spin-resolved properties. Together, these results provide a microscopic understanding of how chirality manifests across the lattice, optical, and spin degrees of freedom. Building on this foundation, we outline a future direction linking these effects through electron–phonon coupling, offering new perspectives on the dynamic origins of chiral-induced spin selectivity (CISS) in hybrid perovskites.

1. Pols, M.; Brocks, G.; Calero, S.; Tao, S. Chiral phonons in 2D halide perovskites. Nano Letters 25, 10003 (2025).
2. Driessen, S.; Sarigul Ozbek, S.; Sutter-Fella, C.; Tao, S. Synthesis and growth of solution-processed chiral perovskites. Journal of Physics: Energy 6, 042001 (2024).
3. Pols, M.; Brocks, G.; Calero, S.; Tao, S. Temperature-dependent chirality in halide perovskites. JPCL 15, 8057 (2024).
4. Apergi, S.; Brocks, G.; Tao, S. Calculating the circular dichroism of chiral halide perovskites: A tight-binding approach. Journal of Physical Chemistry Letters 14, 11565 (2023).

Understanding the Role of Molecular Structure, Conformation and Spin Orbit Coupling in Intersystem Crossing of TADF Emitters

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Keywords: TADF, phosphorescence, carbene, organometallic, spin orbit coupling, intersystem crossing, luminescence

In my talk I will discuss our research toward developing emitters for organic LEDs (OLEDs) with two-coordinate carbene-metal-amide (cMa, M = Cu(I) and Au(I)) complexes.[1-2] Our efforts have been aimed at achieving very short lifetimes (and high Φ_{PL}).[3-4] The cMa complexes studied here emit via thermally assisted delayed fluorescence (TADF) and the TADF lifetime are tied directly to the S_1 decay rate (k_{S1}) and the equilibrium constant for $T_1 \rightleftarrows S_1$ (K_{eq}) and K_{eq} is tied to the energy difference between S_1 and T_1 (ΔE_{ST}).[5] Achieving fast phosphorescence involved designing cMa complexes with small ΔE_{ST} (20-40 meV) while maintaining a k_{S1} in the 10^8 s^{-1} regime. I will discuss how ligand and metal ion choices impact these parameters and the application to OLEDs.

I will also explore the role of spin–orbit coupling (SOC) in facilitating intersystem crossing (ISC) in cMa complexes. Prior studies have shown that ISC rates in these systems span a wide range (10^9-10^{11} s^{-1}).[1] However, the precise contribution of SOC to ISC, and its interplay with TADF, is not well understood. Using a combination of transient absorption spectroscopy, lifetime measurements, and theoretical modeling, we investigate how structural modifications in cMa influences SOC constants (SOCCs). Through Arrhenius and Marcus–Hush theories, we experimentally determined that substituting Cu with Au increases the SOCC from ~2 cm^{-1} to ~7 cm^{-1}, respectively, in agreement with the enhanced ISC rates. Further modifications to the ligands also lead to notable changes in SOCC values. Initial modeling studies suggest that the SOC is greatest for dihedral angles between the carbene and amide ligands near 45°. I will tie these SOC studies back to the observed photophysical properties of both long and short lived cMa complexes. These studies are expected to impact our understanding of organic TADF materials as well.

[1] M. S. Kellogg, A. R. Mencke, C. N. Muniz, T. A. Nattikallungal, F. Cardoso-Delgado, N. Baluyot-Reyes, M. Sewell, M. J. Bird, S. E. Bradforth, M. E. Thompson, *The Journal of Physical Chemistry C* **2024**, *128*, 6621–6635.
[2] T. Y. Li, S. J. Zheng, P. I. Djurovich, M. E. Thompson, *Chem Rev* **2024**, *124*, 4332–4392.
[3] C. N. Muniz, J. Schaab, A. Razgoniaev, P. I. Djurovich, M. E. Thompson, *Journal of American Chemical Society* **2022**, *144*, 17916–17928.
[4] R. Hamze, S. Shi, S. C. Kapper, D. S. Muthiah Ravinson, L. Estergreen, M.-C. Jung, A. C. Tadle, R. Haiges, P. I. Djurovich, J. L. Peltier, R. Jazzar, G. Bertrand, S. E. Bradforth, M. E. Thompson, *Journal of the American Chemical Society* **2019**, *141*, 8616–8626.
[5] D. S. M. Ravinson, M. E. Thompson, *Materials Horizons* **2020**, *7*, 1210–1217.

Vapor phase deposited perovskites; how to improve the photoluminescence quantum yield?

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Keywords: Perovskite, Photoluminescence, Vacuum Deposition

Vapor phase deposited perovskites, suffer from relatively low photoluminescence quantum yield. This limits the external electroluminescence that can be obtained when these perovskites are integrated in diodes. As a result the open circuit voltage when operating as a photovoltaic device is low, and the external quantum yield of electroluminescence is low when operating as an LED. The effect of moderate vacuum deposition methods, such as close-space sublimation on the perovskite luminescent properties will be discussed. We have used in-situ photoluminescence to monitor the photoluminescence evolution of the perovskite film during its vacuum deposition which has enabled us to prepare photovoltaic devices with power conversion efficiencies above 23 %.

Wearable organic optoelectronics for display and healthcare applications

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Rich optical properties and process compatibility of organic semiconductors with various unconventional substrates make organic optoelectronics attractive for wearable consumer devices, which may find applications in stretchable displays and health-monitoring sensors. This talk will provide several successful examples where organic light-emitting diodes (OLEDs) and/or organic photodiodes (OPDs) are employed to realize such wearable healthcare devices with dedicated purposes. They include but are not limited to: (i) ultrathin OLEDs integrated onto a contact lens to measure electroretinography, replacing a bulky Ganzfeld light source for convenient, personalized monitoring of retinal health [1]; (ii) annular OPDs enabling efficient, real-time measurement of carbon dioxides from breath [2]; (iii) multi-junction vertically-stacked OLEDs and OPDs for wearable pulse oximeters with low power consumption and low brightness operation [3]. In addition, this talk will further explore their use in stretchable displays and will discuss what we need to further engineer to build ideal stretchable displays featuring high pixel-density, compensation of resolution loss upon strain, and distortion-free expansion [4,5].

[Keywords] Stretchable Displays, Wearable Healthcare, OLED Contact Lenses, Organic Pulse Oximeters, Carbon Dioxide Sensing,

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References:

[1] J. H. Sim et al., *ACS nano*, 19, 17478, (2025.)
[2] M. Kim et al., *Device*, 3, 100681 (2025).
[3] D. Choi et al., *npj Flexible Electronics*, 9, 26 (2025).
[3] D. Lee et al., *Nature Communications*, 15, 4349 (2024).
[5] S.-B. Kim et al., *Nature Communications*, 15, 7802 (2024).

Active conducting polymer metaoptics

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The redox-tunable properties of conducting polymers make them attractive not only for traditional optical applications like electrochromics, but their ability to switch between metallic and dielectric behavior has also opened unique opportunities for organic tunable plasmonic nanoantennas and metaoptics [1]. After briefly introducing the basics and history of this new area, we will focus on two key challenges: (1) limited performance due to high losses and (2) difficulty in achieving operation in the visible due to limited charge carrier density compared to traditional metals. For the first challenge, we show that careful nonlocal coupling between nanooptical antennas can reduce losses and provide around ten times improved performance in terms of resonance quality factor, making the systems of real practical relevance by also significantly improving signal strengths and modulation depths [2]. For the second challenge, we introduce two concepts enabling operation in the visible, either based on a “conducting polymer optical gate” which dynamically control an optical lattice [3] or a new type of electrochemically tunable metaatom enabling dynamic phase-gradient metasurfaces, where we demonstrate both tunable beam deflection and erasable and rewritable holograms.

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References

S. Chen, E. S. H. Kang, M. S. Chaharsoughi, V. Stanishev, P. Kühne, H. Sun, C. Wang, M. Fahlman, S. Fabiano, V. Darakchieva and M. P. Jonsson, Nature Nanotechnology 15, 35-40 (2020)

D. Lin, Y. Duan, P. Bandaru, P. Li, M. S. Ansari, A. Y. Polyakov, J. Wilhelmsen, and M. P. Jonsson, Nature Communications 16, 4484 (2025)

D. Lin, Y. Duan, S. Kazi, and M. P. Jonsson, Advanced Materials, 38, 10, e20674 (2026)

Anti-Kasha Emission in Difluorenothiophene Diradicals: Impact of Donor-Acceptor Substitution

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Kasha´s rule dictates that the emitting level of a given multiplicity is the lowest energy excited state of that multiplicity. While most fluorophores adhere to this principle, “anti-Kasha” emitters-which bypass this relaxation pathway-offer unique deactivation channels that are highly sought after for advanced optoelectronic applications.[1] Despite their potential, the structural requirements for achieving anti-Kasha behavior remain poorly understood. Expanding on our previous research into difluorene derivatives [2], [3], we report a series of donor/acceptor (D/A)-substituted difluorenothiophene diradicals that exhibit anti-Kasha emission. Our photophysical analysis demonstrates how D/A substitution controls the population and radiative decay of higher-order excited states. Notably, we observed a strong solvatochromic effect linked to the biradical character of the emitting state suggesting a “sudden polarization” mechanism. These findings establish critical structure-property relationships and provide a roadmap for designing environment-sensitive molecular probes and photonic materials.

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References
[1] Zhang, X. et al, Nat. Commun., 15, 2684 (2024)

[2] Moriyasu, R. et al, Chem. Sci., 14, 13468-13474 (2023)

[3] Mori, S. et al, Angew. Chem. Int. Ed, 61, e202206680 (2022)

CdSe Quantum Dots for Interface Passivation in Perovskite Solar Cells

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Perovskite solar cells (PSCs) have emerged as highly promising next-generation photovoltaic devices owing to their high power conversion efficiencies, tunable bandgaps, and excellent light-harvesting properties. However, their broader implementation remains limited by insufficient long-term operational stability, which is strongly affected by surface and interfacial defects acting as non-radiative recombination centers.[1] In this work, CdSe quantum dots (QDs) were investigated as interfacial passivating agents for perovskite films and PSCs. CdSe QDs were synthesized via a hot-injection method using different Cd:Se precursor ratios (1:1, 1:2, and 1:4) to evaluate the influence of composition on nanocrystal growth, optical properties, and passivation behavior. Optical monitoring during synthesis revealed QD sizes ranging from approximately 2 nm at short reaction times to about 5 nm at longer reaction times, with ~3 nm particles identified as the most promising candidates for interfacial modulation. After deposition onto perovskite films, the QDs induced a systematic blue shift in the *in situ* photoluminescence response of the perovskite, and the magnitude of this shift increased with selenium content. These findings suggest that Se-rich CdSe QDs exert a stronger effect on the perovskite/QD interface, supporting the hypothesis that CdSe QDs can reduce interfacial defects and modulate carrier recombination pathways. In addition, preliminary device results showed that CdSe-passivated cells exhibited improved open-circuit voltage (Voc), short-circuit current density (Jsc), and power conversion efficiency (PCE) relative to the control devices, indicating that CdSe incorporation promotes more efficient interfacial defect passivation and charge collection. Overall, these results highlight the potential of CdSe QDs as passivating materials for more stable and efficient PSCs.

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References
Aftab, S. et al. Chemical Engineering Journal vol. 480 (2024).

Coinage Metal TADF Emitters for Stable OLEDs and Nonlinear Photonics

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Two-coordinate coinage metal complexes with linear geometry L–M–X (L = carbene and X = anionic ligand, M = copper, silver or gold) have recently emerged as a new class of strongly photoemissive materials – Carbene Metal Amides (CMA). We will discuss the advances in CMA molecular design to cover the full visible spectrum and near-IR region (up to 850 nm). Advanced deep-blue gold CMA emitters will be demonstrated to have radiative rates approaching 107 s-1 [1]. CMA OLEDs with significantly improved device lifetimes, for instance, the red CMA OLED with LT95 reaching 195 h @1000 cd m-2, will be presented to demonstrate the promising molecular design concepts and the applied potential of the new CMA materials. A comprehensive comparison across various classes of emitters will be based on the bond dissociation energies of the metal–ligand bond and on intra- and intermolecular contacts in the CMA emitter, to demonstrate molecular designs that lead to the best photophysical and OLED performance. For instance, the role of strong agostic and weak anagostic C–H□M intramolecular interactions will be correlated with non-radiative events, as supported by gas-phase photoluminescence [2] to highlight the impact on the photophysics and future molecular design. CMA molecular design towards bright fluorescence, phosphorescence, TADF, and energy-transfer OLEDs will be covered, including the latest results on host-free CMA OLEDs and proof-of-principle anti-Kasha electroluminescence with narrowband emission (FWHM 26 nm). The first CMA material will be demonstrated to exhibit enhanced two-photon absorption (2PA cross-section up to 105 GM) and bright red 2P-TADF with excellent photostability, encouraging further CMA exploration for future applications that require third-order nonlinear optical properties [3].

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References

A.C. Brannan, Adv. Sci. 13(6), e16582 (2026).

A. Belyakov. Chem. Commun., 61, 19104 (2025).

I.D. Nwosu, Commun. Chem. (2026); https://doi.org/10.1038/s42004-026-01928-5

Control of the photoluminescence quantum yield of noble metal organometallic nanocomposites by pulsed laser driven CO_2 reduction reaction

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In recent years, there has been a huge interest in the CO2 reduction reaction (CO2RR) for the production of value-added raw materials in gas or liquid form. However, CO2 fixation into nanoparticle systems has not yet been demonstrated. This research presents a novel approach to control the photoluminescence of noble metal (gold, silver) organometallic nanoclusters by the pulsed laser driven CO2 fixation in water [1]. This novel environmental friendly approach, allows the in-situ generation of organic material from the laser driven CO2RR, which interacts with metal clusters obtained through the ablation process, allowing their stabilization and relative control of the photoluminescence quantum yield of almost one order of magnitude.

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References
Tahir et al., "Pulsed laser driven CO2 reduction reaction for the control of the photoluminescence quantum yield of organometallic gold nanocomposites", Small Science, Volume 4, Issue7, 2024, 2300328. https://doi.org/10.1002/smsc.202300328

Controlling Nanoscale Interfacial Reorganization to Extend Electrochemiluminescent Device Lifetime

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Soft, low-temperature processed organic light-emitting devices are highly desirable for flexible and large-area photonics. However, they typically rely on complex multilayer thin-film architectures that complicate fabrication. Electrochemiluminescent devices (ECLDs) offer a structurally simpler single-layer alternative, yet their operational lifetime under AC driving remains critically limited—stable emission often ceases within minutes [1]. Here, we demonstrate that device performance and durability are fundamentally governed by nanoscale electrolyte–electrode interfacial energetics, specifically the restructuring dynamics of the electric double layer (EDL). By replacing the bulky $[TFSI]^-$ anion with the more compact, we lower interfacial reorganization barriers and facilitate faster ion rearrangement near the electrode. This accelerates EDL resetting, yielding shorter non-emissive intervals, faster emission rise times, and enhanced luminance stability. The optimized system achieves sustained operation at elevated frequencies and an extended lifetime ($L_{50} \approx 117$ min) under potentiostatic AC control—an order-of-magnitude improvement over baseline. Notably, these gains are realized on transparent FTO electrodes, eliminating the need for costly gold electrodes or galvanostatic driving [2, 3]. This work establishes that rational nanoscale interfacial design through anion engineering can substantially enhance operational stability while preserving single-layer simplicity, offering a direct pathway toward robust, low-cost hybrid organic light-emitting systems.

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References

Chen, Z., Xu, H., Pan, C., & Bao, R. (2025). Electrochemiluminescent devices: Structural composition, preparation process and applications for flexible/stretchable displays. Wearable Electronics, 2, 149-170.

Yee, H., Lee, J. I., Park, D. M., Jung, K., Lee, S., Kim, N. H., ... & Kang, M. S. (2024). Extending the operational lifetime of electrochemiluminescence devices by installing a floating bipolar electrode. Small, 20(15), 2307190.

Yee, H., Jung, K., Park, J., Choi, W., Kim, N. H., Kim, J., & Kang, M. S. (2025). Transparent Electrode-Free Light-Emitting Devices Exploiting Ion Transport-Controlled Electrochemiluminescence. Advanced Functional Materials, 35(14), 2417514.

Degradation study of red hyperfluorescent OLED devices based on TXO-TPA and DBP as TADF assistant and fluorescent emitter respectively

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In recent years, there have been efforts from both academia and industry to bring the Thermally Activated Delayed Fluorescence (TADF) materials to the Organic light-emitting diodes (OLED) market [1]. These materials were first designed as the light-emitting material in OLED devices due to their efficient exciton utilization using the reverse intersystem crossing (RISC) mechanism which allows the reconversion of non-emissive triplet excitons into emissive singlet excitons, allowing for a potential 100% exciton utilization. However, these TADF materials have non-saturated colour emission, which is detrimental for full-colour applications. Hyperfluorescence emerged as a solution by incorporating a third component in the emissive layer, namely a fluorescent emitter [2]. In these devices, the TADF material can convert generated triplet excitons into singlet excitons and then transfer all the singlet excitons to the fluorescent emitter material. This allows for efficient exciton harvesting by the TADF molecule while obtaining a saturated colour emission from the fluorescent emitter, achieving highly efficient emission [3]. However, there has been less focus on the study and report of the lifetime of these devices and the knowledge of the degradation mechanisms of the organic materials used therein. In this work, a red hyperfluorescent OLED device based on the TADF molecule TXO-TPA and the red fluorescent molecule DBP is used as a model for the study of OLED degradation. Current-voltage-luminescence curves and external quantum efficiencies (EQEs) were obtained at different operating times, allowing for lifetime operation monitoring

Acknowledgements
FONDECYT Postdoctoral Grant No. 3250646

References

Dos Santos, J. M. et al. The Golden Age of Thermally Activated Delayed Fluorescence Materials: Design and Exploitation. Chem. Rev., 124, 13736–14110 (2024)

Nakanotani, H. et al. High-efficiency organic light-emitting diodes with fluorescent emitters. Nat. Commun., 5, 1–7 (2014)

Aarti, et al. Recent Progress and Challenges in Molecular Design for Hyperfluorescent Based Organic Light Emitting Diodes (OLEDs). Adv. Optical Mater., 13, e01648 (2025)

Donor-dependent photophysical pathways in Organic bulk heterojunction solar cells

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The performance of organic bulk heterojunction (BHJ) solar cells relies on the interplay between donor and acceptor materials to drive efficient charge generation and transport [1]. While the non-fullerene acceptors attract wide research interest [2], the influence of the donor polymer on shaping ultrafast excited-state dynamics remains less understood. In this work, we investigate four donor polymers- PTQ11, PM6, D18, and PDPP3T- in blends with the common acceptor L8-BO, to understand how donor selection affects the photophysical pathways underlying device performance. The corresponding solar cells exhibited significantly different power conversion efficiencies, suggesting distinct charge generation and loss mechanisms across the blends. Femtosecond transient absorption spectroscopy was employed in the visible and near-infrared regions to capture the ultrafast excited-state processes and charge generation. By correlating transient spectral signatures and kinetic profiles with device performance metrics, we identified notable donor-dependent variations. The device with PDPP3T:L8-BO blend with the lowest energy offset performed the worst in terms of efficiency. The other three blends with the better device performances showed sub-picosecond energy transfer from the donor to the acceptor and they exhibited efficient exciton dissociation, formation of the intermediate charge-transfer states and charge formation. From the spectra, excitons and charge species were effectively deconvoluted to further resolve the charge-generation pathways. Such insights are useful for proper donor selection for optimizing L8-BO and other non-fullerene acceptors-based BHJ solar cells, and improving understanding of next-generation high-efficiency organic photovoltaics.

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References

Omar A. Abdulrazzaq , Viney Saini, et. al., 31:5, 427-442(2013)

Dou Luo, Woongsik Jang, et. al., 10, 3255(2022)

Electrochromic Smart Windows: Achieving an Absolute Private State through Thermochromically Engineered Electrolyte

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Smart windows regulate the indoor solar radiation by adjusting their optical transmissive properties from transparent to deeply colored state,[1,2] offering an efficient way toward energy-saving buildings, vehicles, etc. Electrochromism is one of the most promising solutions due to its simple control, versatile colors. Yet, electrochromics cannot give zero-transmission through the whole visible range, leading to the windows that can always be looked through and limited for applications in the public sector. In this work, poly(N-isopropylacrylamide) (PNIPAm) hydrogel, which undergoes temperature-stimulated phase transition from a highly transparent state to a highly scattered zero-transmission state through the whole visible range was used in the electrolyte of the electrochromic devices without affecting their electrochromic performance.[3] We showed that it can be universally applied to inorganic and organic electrochromic devices, and the phase transition temperature can be easily tuned by the ion concentration. Therefore, apart from its ion conductive function, the electrolyte performs the chromatic transition function, allowing the electrochromic devices to achieve a zero-transmissive, absolute “private” state. This chromatic engineering of the electrolyte can significantly broaden the industrial market of electrochromic smart window applications from public to private circumstances and bring much more flexibility in building facades design, which is a remarkable pavement for further industrial applications.

References

W. Li et al. Polym. Chem., 2018, 9, 5608

D. Chen et al., Nat. Commun. 2024, 15, 8457

M. Wang et al., Adv. Energy Mater. 2019, 9, 1900433

Engineering Delayed Emission in Phenanthrene Diketal Emitters for OLEDs

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Phenanthrene diketal derivatives represent a promising platform for tuning excited-state processes in purely organic OLED emitters. In this work, we investigate a family of phenanthrene-9,10-di(ethylene) diketal compounds comprising the donor-free reference dKet0 and four donor-substituted derivatives bearing phenoxazine or phenothiazine units. This molecular design enables direct comparison of donor type, substitution pattern, and host-matrix effects within a single compact scaffold. Photophysical studies reveal that delayed emission in these materials is highly sensitive to the surrounding environment. In solution, the donor-substituted compounds exhibit broad, solvent-dependent emission, indicating mixed excited-state character. In rigid matrices, time-resolved measurements show that Zeonex mainly supports fluorescence-like delayed emission, whereas CBP promotes phosphorescence-dominated delayed emission. Temperature-dependent experiments further indicate the involvement of multiple triplet states in the emissive process, highlighting the complex interplay between locally excited, charge-transfer, and triplet-state manifolds. In contrast, the donor-free reference does not exhibit comparable delayed fluorescence, confirming the key role of donor–acceptor coupling in enabling efficient triplet harvesting. A clear regioisomer effect is also observed, with the 2,7-substituted derivatives outperforming the corresponding 3,6-substituted analogues in both photophysical response and OLED performance. Devices fabricated using CBP as the host confirm that controlled molecular engineering of the diketal framework translates into efficient electroluminescence. Overall, these results demonstrate that phenanthrene diketal emitters constitute a versatile platform for engineering delayed emission pathways and provide useful design guidelines for the development of next-generation OLED materials.

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References
none

Evaluation of Molecular alignment, Mobility, and Photodiode Characteristics in Liquid Crystalline Organic Semiconductor Bulk Heterojunction Films

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Liquid crystalline diketopyrrolopyrrole and fullerene derivatives (DmPP-O12:PC61BM) bulk heterojunction (BHJ) films exhibit a vertical orientation of DmPP-O12 molecules after spin-coating. However, thermal annealing at 60 °C of crystal phase following top electrode fabrication induces planar orientation[1]. Same as DmPP-O12, the molecular alignment of DmPP-O10, which has a different alkyl chain length also changes from vertical to planar orientation after thermal annealing. This study reports on the spontaneous orientation change of DmPP-O10 in the BHJ films without thermal annealing. DmPP-O10:PC61BM was mixed in a 2:1 weight ratio and dissolved in chloroform, spin-coated to fabricate BHJ film. Samples were stored at room temperature (approximately 20°C). Organic photodiodes (OPDs) were fabricated in an inverted structure using poly(ethyleneimine)/ITO and MoO3/Au electrode. Polarized optical microscopy (POM) images revealed that the BHJ film exhibited no retardation after spin-coating, suggesting vertical orientation of DmPP-O10 molecules. However, bright-field regions, suggesting planar orientation, expanded over time. The entire area exhibited bright-field 96 hours after spin-coating. This change in POM images correlated with the results from out-of-plane wide-angle X-ray diffraction patterns. The responsivity of the fabricated OPD increased from 23 mA/W to 150 mA/W at a wavelength of 560 nm after 96 hours. The increase in responsivity was attributed to improved mobility due to orientation changes of DmPP-O10 and suppression of bimolecular recombination. The mobility obtained by charge extraction by linearly increasing voltage in metal-insulator-semiconductor (MIS-CELIV) method increased from 4.4×10-7 cm2/Vs (12 hours post-spin-coating) to 7.5×10-5 cm2/Vs (96 hours post-spin-coating). These results indicate that spontaneous orientation changes of liquid crystalline diketopyrrolopyrrole derivatives in BHJ films significantly improves mobility and OPD performance.

References

K. Nakano et al. Apl. Phys. Express 5, 111701 (2012).

From Interface to Bulk: Hierarchical Integration of Quantum Dots in Perovskite Solar Cells

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Despite their impressive power conversion efficiency, interfacial defects and ion migration phenomena continue to restrict the operational stability of perovskite solar cells (PSCs). We present three quantum dot (QD)-based strategies that simultaneously address ionic dynamics and interfacial recombination in metal halide perovskites (MHPs). First, CdS QDs are introduced as a buried interlayer between SnO_2 and the perovskite absorber. This approach reduces surface oxygen vacancies and hydroxyl groups on SnO_2, as confirmed by XPS, while KPFM mapping reveals improved homogeneity of surface potential. Perovskite films grown on CdS-passivated substrates exhibit enhanced crystallinity and charge extraction, resulting in ~15% higher efficiency and improved stability under ISOS-D-1 conditions.1 Second, perovskite QDs are employed to passivate the top MHP/HTL interface. Using in situ PL spectroscopy, we track halide exchange reactions at the 3D/QD heterojunction and extract the activation energy for Br-to-I exchange. This process suppresses bimolecular recombination and improves interfacial energetics, enhancing hole extraction and thermal stability.2 Finally, we demonstrate that lateral ion migration is influenced by embedding PbS QDs in perovskite films. PbS QDs act as local ionic interaction centers, modifying halide redistribution pathways and increasing the activation energy required for lateral ionic transport, based on electrical and spectroscopic analyses. This can enhance operational stability and decrease field-induced degradation by preventing ion buildup under bias and illumination. All of these findings indicate that quantum dots act as active modulators of ionic dynamics and as interfacial passivators, opening new possibilities for nanoscale ionic engineering to stabilize PSCs.

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References

Fonseca, A. F. V. da; Germano, G. M.; Scalon, L.; Almeida, C. A. N.; Barra, Á. C. C.; Ribeiro, D. S.; al., et. CdS Quantum Dot Interlayer Engineering for Enhanced SnO_2/Perovskite Interfaces in Solar Cells. ChemRxiv. https://doi.org/10.26434/chemrxiv-2025-t6j9k-v3

Fonseca, A. F. V.; Scalon, L.; Vale, B. R. C.; Guaita, M. G. D.; Bettini, J.; Brandão, Z. C.; Zagonel, L. F.; Padilha, L. A.; Nogueira, A. F. In Situ PL Tracking of Halide Exchange at 3D/QD Heterojunction Perovskite Solar Cells. ACS Energy Lett. 2024, 9 (6), 3177–3186.

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Herzberg–Teller Effect as a Phonon-Assisted Optical Transition

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Fluorescence generally occurs when the electric dipole transition between initial and final states is symmetry allowed. However, even if the transition is symmetry-forbidden, fluorescence can occur due to the symmetry breaking associated with molecular vibration. This is called the Herzberg-Teller effect in fluorescence, which has recently attracted attention as an application to OLEDs. In this study, we employ the crude adiabatic representation (Longuet-Higgins representation), where the role of vibronic coupling is more straightforward than the Born-Oppenheimer representation, to formulate the Herzberg-Teller effect. Then, we show that the Herzberg-Teller effect can be described as a phonon-assisted fluorescence, enabling us to clarify the quantitative relationship between transition and vibronic coupling of all molecular vibrational modes. Combined with density functional theory calculations, the vibronic structures responsible for the Herzberg-Teller effect in the anti-Kasha fluorescence of azulene are revealed.

Acknowledgements
JP24K23082, JPMJAP2334

References

W. Ota, M. Uejima, T. Sato, Bull. Chem. Soc. Jpn. 96, 582 (2023).

W. Ota, M. Uejima, N. Haruta, T. Sato, Bull. Chem. Soc. Jpn. 97, uoad020 (2024).

A. Nakagawa, Wataru Ota, T. Ehara, Y. Matsuo, K. Miyata, K. Onda, T. Sato, S. Seki, T. Tanaka, Chem. Commun. 60, 14770 (2024).

High-Mobility, Short-Lifetime Organic Emitters Enabling High-Speed Modulation in OLEDs for Visible Light Communication

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Organic light emitting diodes (OLEDs) are now widely incorporated in display, lighting, and several smart devices. This adoption can be complimented with several new applications such as optical data transfer among devices, time-resolved fluorescence measurements of biomarkers, and secure visible light communications (VLC). These applications demand fast modulation (temporal performance) of OLEDs which are intrinsically slow due to low charge mobility and long fluorescent lifetimes of organic materials, and high resistance-capacitance (RC) in the devices.1 There has been increasing attention towards the exploration of organic materials and device architectures for the development of fast OLEDs1-3. However, further progress and effort to develop emitter materials with high charge-mobility, short fluorescent lifetimes, and complementing device structures is essential to address the demands of high-bandwidth VLC. Herein, we present the development of new fluorene-based organic emitters designed to meet the challenging criteria of VLC. The high charge (electron and hole) mobilities (~10-3), short fluorescence lifetimes (<5 ns), quantum yield of over 50%, and high glass transition temperatures (>120°C) makes these emitters suitable candidates for the application. These emitters were then employed to explore the OLED device designs with an aim to reduce the RC-time of the devices. Device architectures with neat emitter layer (EML), host-guest EMLs with varying emitter concentrations combined with changing the characteristics of the charge transport layers provided valuable insight into the route towards development of fast-modulation OLEDs. As a result, OLEDs with state-of-the-art bandwidths reaching 300 MHz were developed. The work presents a route and understanding towards the development of next generation of materials and OLEDs capable of fast modulation suiting the needs of communications applications.

Acknowledgements
HORIZON EIC Grants for High-Speed Organic Photonics and OptoElecronics (HiSOPE) project

References
1) Yoshida, K., Manousiadis, P.P., Bian, R. et al. 245 MHz bandwidth organic light-emitting

diodes used in a gigabit optical wireless data link. Nat Commun 11, 1171 (2020).

2) Munshi N. M., Loganathan N., Chakaroun M., et al. High-speed OLED bandwidth optimisation method based on Relative Intensity Noise measurements. Org Elect, 123, 106935 (2023)

3) Yoshida, K., Chen C., Haas H., et al. RGB-Single-Chip OLEDs for High-Speed Visible-Light Communication by Wavelength-Division Multiplexing. Adv Sci 11:47, 2404576 (2024)

How Multiple RISC Pathways Shape Efficiency and Roll-off in TADF OLEDs

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Thermally activated delayed fluorescent (TADF) emitters are promising for high-efficiency OLEDs, but the link between molecular structure, excited-state dynamics, and device performance, particularly device roll-off, is still not fully understood [1]. In this talk, I will present a photophysical study of a family of multidonor–acceptor TADF emitters, showing how donor–acceptor dihedral angles influence HOMO–LUMO separation, singlet–triplet energy gaps, and the distribution of charge-transfer and local triplet states. These effects give rise to multiple reverse intersystem crossing (rISC) pathways, which are strongly host-dependent. By correlating these pathways with OLED performance, we show that fast rISC supports external quantum efficiencies above 20%, while slower rISC channels act as parasitic traps that drive severe efficiency roll-off. This explains why some emitters combine excellent peak efficiency with poor roll-off, and highlights the importance of both molecular design and host environment in TADF OLED performance. Using this analysis, we can predict device roll-off from the photophysics by examining the dispersion of emissive states [2].

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References

Larissa G. Franca, David G. Bossanyi, Jenny Clark, Paloma Lays dos Santos, ACS Appl. Opt. Mater. (2024)

Paloma Lays dos Santos, Daniel de Sa Pereira, Chan Seok Oh, Nadzeya Kukhta, Ha Lim Lee, Jun Yeob Lee, Andrew P. Monkman, J. Phys. Chem. C , 128, (2024)

Light-Induced True Random Number Generation in Bipolar Photo-Responsive Devices for Hardware Deepfake Security

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We present a light-induced hardware true random number generator (TRNG) and authentication scheme based on a bipolar photo-responsive photodetector (BPPD) architecture that exploits intrinsic material disorder and wavelength-dependent photocurrent polarity inversion under optical excitation. The proposed device uses polychromatic illumination, including deep-ultraviolet (DUV) and blue light, to generate distinct positive and negative photocurrents without external bias, enabling robust entropy extraction from physical processes. The BPPD's material and structural disorder, combined with asymmetric carrier generation under different wavelengths, produce highly stochastic photocurrent distributions. These light-induced currents are mapped to binary bit streams that satisfy multiple randomness quality metrics, including uniform bit distribution (~50%), high entropy, and independence, as confirmed by NIST SP 800-22 statistical tests on ≥460,000 bits. A custom readout circuit achieves a sustained ~2 kbps true random bit output, which is then demonstrated in a wireless random number transmission setup. This material-enabled light-polarity contrast mechanism provides a robust physical entropy source that is inherently resilient to algorithmic predictability and cloning. Unlike conventional pseudo-random or solely electronic noise sources, the proposed optoelectronic TRNG generates device-unique randomness useful for hardware authentication and deepfake detection at the sensor layer, where physical signatures can distinguish genuine signals from AI-generated synthetic media. Integration of optical randomness into hardware security primitives offers a pathway toward secure edge computing and trustworthy artificial intelligence applications.

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References
"Rolling the Dice with Light Competition: Introducing a True Random Number Generator Powered by Photo-Induced Polarity Current." Advanced Materials 37.14 (2025): 2419579.

Materials to enable new-generation photovoltaics at industrial scale

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Achieving carbon-neutral energy production requires a rapid increase of electricity production using solar energy. To achieve this goal, new generation organic (OPV) and perovskite photovoltaics are needed. Technologies which are currently under development include: a) tandem approaches combining conventional, e.g., silicon solar PV, with Perovskite-based solar cells, b) single- and multi-junction perovskite but also organic photovoltaic devices for the energy- and cost-efficient manufacturing on light-weight flexible substrates [1] , and c) OPV devices optimized for operation under low light conditions, targeting, particularly, IoT applications. Both organic and perovskite photovoltaics require the industrial availability of materials with specific electronic, physical and chemical characteristics. The optimization of the properties of unfunctionalized fullerenes (especially C60), available at industrial scale for vapor deposition, will be described [2]. The selection and design of organic materials to be used in the active layer of high performing OPV and in the interlayers of n-i-p and p-i-n perovskite PV devices will be discussed. The importance of functional groups suitable to form self-assembled monolayers (SAM) and/or stabilize the perovskite phase will be assessed. Fullerene derivatives, e.g., bearing phosphonic acid or amino-/ammonium-groups will be presented. Addressing the need for improved hole transport materials (HTM) for Perovskite PV, molecules with suitable electronic properties such as triphenylamines and carbazoles bearing, e.g., phosphonic or boronic acid will be described. Innovative concepts, such as the use of cross-linking or the presence of more than one functional group to improve the quality but also stability of interface layers are explored. Fully optimized OPV stacks targeting a power conversion efficiency of 10% under 1 SUN at module level, will be shown. Thermal and light soaking stability data will be reported.

References

[1] J. Han, K. Park, S. Tan, Y. Vaynzof, J. Xue, E. Wei-Guang Diau, M. G. Bawendi, J.-W. Lee and I. Jeon, Nat. Rev. Methods Prim. 5, 3 (2025).

[2] A. A. Said, E. Aydin, E. Ugur, Z. Xu, C. Deger, B. Vishal, A. Vlk, P. Dally, B. K. Yildirim, R. Azmi, Jiang Liu, E. A. Jackson, H. M. Johnson, M. Gui, H. Richter, A. R. Pininti, H. Bristow, M. Babics, A. Razzaq, S. Mandal, T. G. Allen, T. D. Anthopoulos, M. Ledinský, I. Yavuz, B. P. Rand and S. De Wolf, Nat. Commun. 15 (2024), 708 (2024).

Mobility imbalance as a design paradigm for ultrafast organic photodetectors in optical communication

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Organic photodetectors (OPDs) offer intrinsic advantages such as spectral tunability and mechanical flexibility, enabling emerging applications in wearable sensing and integrated optical communication. However, their bandwidth is fundamentally limited by low charge carrier mobility, which is conventionally addressed through balanced electron and hole transport. Here, we demonstrate an alternative strategy based on controlled mobility imbalance within bulk-heterojunction OPDs. By comparing mobility-balanced ($\mu_e \approx \mu_h$) and strongly imbalanced ($\mu_e >> \mu_h$) systems, we show that the presence of ultrafast majority carriers can dominate the transient extraction dynamics. The device exhibits an electron mobility of 0.1 $cm^2 \cdot V^{-1} \cdot s^{-1}$, nearly three orders of magnitude higher than the hole mobility (1.3×10^{-4} $cm^2 \cdot V^{-1} \cdot s^{-1}$), resulting in rise/fall times of 3.7 ns/43.1 ns, respectively, and a 22 MHz cutoff frequency at 0 V. Drift–diffusion simulations combined with time-resolved photocurrent measurements reveal an initial recombination-free electron extraction process followed by slower recombination-mediated hole transport. The mobility-imbalance-induced space-charge region (SCR) enhances bandwidth at the expense of photocurrent amplitude, exposing the limitations of conventional speed metrics that overlook signal strength. To quantify this trade-off, we introduce the transient dynamic range (TDR) as a figure of merit capturing both signal magnitude and slew rate for optical communication. Eye-diagram analysis confirms suppressed overshoot and undershoot behavior, enabling reliable data transmission at 170 Mbps (BER < 10^{-3}), outperforming the mobility-balanced devices by an order of magnitude. The device further achieves a specific detectivity (D*) of 1.8×10^{14} Jones at 405 nm (−4 V). These results redefine OPD design principles by demonstrating that controlled mobility imbalance combined with SCR engineering enables ultrafast OPD for high-performance optical communication.

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References

S. Wilken, O. J. Sandberg, D. Scheunemann, and R. Österbacka, Sol. RRL, 4, 1900505 (2020)

Modeling Environmental Effects on the Electronic Properties of Bulk Heterojunctions for Organic Solar Cells

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Understanding the optoelectronic properties of bulk heterojunction (BHJ) thin films remains a key challenge in the development of high-efficiency organic solar cells. In this work, we extend our multiscale simulation protocol, previously applied to donor-acceptor systems such as PF5-Y5 and later to non-fullerene acceptor films including Y6, to the study of state-of-the-art BHJ blends based on PM6 combined with Y6 and L8-BO. Our multiscale approach is based on a sequential QM/MM framework in which the system is first described through classical molecular dynamics simulations, employing an evaporation protocol to transition from solution to thin-film conditions, followed by electronic structure calculations on representative snapshots using a QM/MM approach. In this framework, environmental effects were described either through continuum models employing experimental dielectric constants or through a polarizable electrostatic embedding scheme that does not require prior knowledge of macroscopic dielectric properties, representing a significant advancement for theoretical modeling of complex organic materials where such data are often scarce. We focus on the characterization of key optoelectronic features, including UV-Vis absorption spectra and the nature of low-lying excited states, providing a picture of how molecular packing and local environments influence the electronic structure in these complex materials. Notably, we observe differences in the excited-state character arising from the anisotropic nature of the thin films, which are captured by the electrostatic embedding description of the environment. In addition, we present, for the first time, results obtained using the polarizable embedding framework for BHJ systems. Our findings demonstrate the capability of multiscale approaches to bridge realistic film structures and excited-state properties, offering new insights into the understanding of next-generation organic solar cells.

Acknowledgements
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References
L. R. Franco, D. Valverde, C. Marchiori, E. Moons, E. Wang, C. M. Araujo, Journal of Physics: Energy 7, 045001 (2025)

Nanostructures for efficient organic light-emitting diode emission management

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OLEDs are increasingly applied in illumination and displays because they offer excellent color quality, are mechanically flexible, and are self-emissive. Their usage is, however, limited by their low external quantum efficiency and efficiency roll-off at high driving voltages. This, together with demands for smaller pixels and device sizes in emerging technologies, motivates innovations that increase efficiency and allow replacing external optical elements used for light manipulation with embedded solutions. Commonly, the research towards outcoupling enhancement in OLEDs focuses on molecular design of the emitters and on various external components, such as Micro Lens Arrays and substrate roughening [1,2]. External components can only be used to extract substrate modes, are often bulky, and expensive to manufacture. Here, we demonstrate enhanced outcoupling as well as directional and polarization control of emission with the inclusion of nanostructures within OLED devices. Unlike the external solutions, the inclusion of nanostructures allows extraction of light from all lossy modes. Furthermore, they are compatible with miniturization demands of the devices. We have realized maximum enhancement of 30% at near-normal directions as well as significant narrowing and blue-shifting of the emission profile. Furthermore, non-trivial nanostructures, that provide angle-independent color of emission, have been studied and shown promise. Lastly, polarization dependent response with a degree of linear polarization, defined via Stokes parameters as S1/S0, has been observed with a ration of 0.3 at the strongest modes.

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References

Möller, S.; Forrest, S. R. Improved Light Out-Coupling in Organic Light Emitting Diodes Employing Ordered Microlens Arrays. Journal of Applied Physics 2002, 91, 3324–3327

Zhou, J.; Ai, N.; Wang, L.; Zheng, H.; Luo, C.; Jiang, Z.; Yu, S.; Cao, Y.; Wang, J. Roughening the White OLED Substrate’s Surface Through Sandblasting to Improve the External Quantum Efficiency. Organic Electronics 2011, 12, 648–653.

Organic electronicsbased on thienothiophene and ditihienothiophene

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Thienothiophene (TT) and dithienothiophene (DTT) are the simplest fused thiophenes, composed of two annulated thiophene rings. TTs and DTTs have extended □-conjugation, planar structure, intermolecular S---S interaction, and electron rich, flat, rigid, and good electron delocalized skeleton. These properties make them very suitable and desirable main building blocks for organic electronics. Thus, they have been attracted a great interest in material chemistry as both polymeric and small molecules for organic electronics such as organic light emitting diodes (OLED), organic field effect transistors (OFET), organic solar cells (OSC), capacitors and sensors. Thanks to the versatile properties of TTs and DTTs, various research groups have focused on TT chemistry, particularly for the development of energy and energy-based smart materials. Our research group is one of the leading one on the development of new synthetic methodologies for the synthesis of substituted TTs and DTTs. Recently, our research group has conducted striking studies on TT and single wall carbon nanotube (SWCNT) based materials. These materials have been obtained without using any binding agents and they have shown remarkable energy storage and supercapacitor performances as flexible, easily bendable and binder-free nanomaterials.

Acknowledgements
Istanbul Technical University, TUBITAK

References

“Thienothiophenes, Dithienothiophenes, and Thienoacenes: Syntheses, Oligomers, Polymers, and Properties” Mehmet Emin Cinar and Turan Ozturk, Chem. Rev., 2015, 115, 3036 - 3140

Protonation-Mediated Delayed Emission in Organic Materials: Dynamic Control of Triplet Excitons via Hydrogen-Bonded Environments

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Delayed emission in organic materials offers a promising route to long-lived luminescence without reliance on heavy metals or crystalline order, yet remains difficult to control in amorphous and processable systems due to weak spin–orbit coupling and efficient non-radiative decay[1,2]. Here we report a distinct class of delayed emission in fused heteroaromatic organic luminophores in which protonation and hydrogen-bond interactions dynamically regulate singlet–triplet coupling. Two constitutional isomers based on a carbazole–pyridine framework were investigated in polymer matrices with contrasting chemical environments. While weak delayed emission is observed in an inert host a controlled pronounced long-lived emission emerges in polar and acidic matrices, with lifetimes ranging from milliseconds to seconds under ambient conditions. Time-resolved photoluminescence reveals a clear separation between prompt fluorescence and delayed emission while time-gated spectra display vibronic resolved features characteristic of triplet-mediated processes[3]. Acid–base modulation experiments demonstrate reversible spectral and kinetic changes, linking delayed emission to protonation-induced reorganization of the excited-state landscape. Protonation stabilizes charge-transfer-like singlet states and introduces low-lying n–π* character, effectively reducing the ΔEST gap, enhancing intersystem crossing and reverse intersystem crossing via spin–vibronic coupling while hydrogen bonding suppresses non-radiative relaxation. Subtle differences in molecular topology lead to markedly different delayed-emission dynamics, highlighting the sensitivity of this mechanism to constitutional isomerism. These results establish hydrogen-bond-mediated protonation as a chemically addressable strategy for controlling delayed emission in organic solids, expanding the design space beyond conventional TADF and room-temperature phosphorescence toward environmentally regulated adaptive luminescent materials

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References

MA, Dian-Xue et al. Nylons with highly-bright and ultralong organic room-temperature phosphorescence. Nature Communications, v. 15, n. 1, p. 4402, 2024.

ZHANG, Xue et al. A class of organic units featuring matrix-controlled color-tunable ultralong organic room temperature phosphorescence. Advanced Science, v. 10, n. 3, p. 2206482, 2023.

PENFOLD, Thomas J. et al. Spin-vibronic mechanism for intersystem crossing. Chemical reviews, v. 118, n. 15, p. 6975-7025, 2018.

Pushing the boundaries of the energy gap law: Near-infrared TADF material spectroscopy

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Near-infrared (NIR) organic light-emitting diodes are highly promising for photobiomodulation (PBM) therapy in neurodegenerative disease management due to their mechanical flexibility. NIR light (700–1400 nm) penetrates deep tissue, and since the optimal wavelength for PBM is undefined, donor-acceptor-donor (D-A-D) thermally activated delayed fluorescence (TADF) emitters are ideal; their broad and tuneable emission covers a large spectral range. However, developing efficient NIR-emitting chromophores is challenging due to the energy gap law. According to this empirical law, when the potential energy gap between two states (e.g. S1→S0) reduces, excitons are more likely couple to the higher vibronic states and decay non-radiatively, rather than by emitting light. Consequently, photoluminescence quantum yield (PLQY) drastically decreases with increasing emission wavelength [1]. Recently, it was shown that optimizing intra and intermolecular charge transfers can enable higher emission wavelengths [2]. Here, we explore the effect of intermolecular inhibiting and promoting donor moieties on a series of twisted D-A-D TADF molecules emitting in the deep red/NIR region. With a 150 nm full-width half maximum emission and a doping controlled peak emission spanning 170 nm, these materials fulfill the requirement for PBM therapy. Notably, these novel molecules emit above 700 nm while maintaining a PLQY above 50%. We observed in solid state that triplet-state energies were more influenced by molecular design, whereas singlet-state energies were comparatively less affected. Nonetheless, all compounds exhibited TADF, with distinct reverse intersystem crossing rates and delayed fluorescence lifetimes. Furthermore, spectroscopic and computational data show steric encapsulation hindered aggregation in one of these materials. Overall, this work establishes donor-moiety engineering as an effective strategy to control intermolecular interactions and optimize NIR TADF emitters for PBM.

References

[1] P. L. dos Santos, P. Stachelek, Y. Takeda, P. Pander, Mater. Chem. Front., vol. 8, no. 7, pp. 1731–1766 (2024)

[2] J. Xu, Y. Dai, J. Zhang, Z. Jia, Q. Meng, J. Qiao, Adv. Opt. Mater., vol. 12, no. 3, p. 2300989 (2024)

Reducing singlet-triplet annihilation losses in hyperfluorescent OLEDS and organic lasers

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Singlet-triplet annihilation (STA) is responsible for significant efficiency roll-off in OLEDs at high luminance, prevents continuous-wave (CW) lasing in solid organic materials under optical pumping and makes realization of electrical pumping very challenging. Losses to STA are particularly severe in OLEDs which use thermally activated delayed fluorescence (TADF) emitters because of long-lived triplet excitons [1]. Dozens of cases of efficient hyperfluorescent OLEDs have also been reported but the roll-off problem still remains. Understanding of the efficiency limiting processes is needed for their mitigation and for designing more efficient materials for hyperfluorescent OLEDs and organic lasers. Here we combine time-resolved luminescence and transient absorption spectroscopies of thin films and of working OLEDs to investigate the processes responsible for efficiency roll-off in hyperfluorescent OLEDs. We show that even with careful selection of TADF sensitizers and terminal emitters, a small fraction of triplet excitons form on the terminal emitter and cause large loss of singlet excitons to STA. We have identified some materials combinations which reduce STA losses and can be used for developing bright hyperfluorescent OLEDs. We also show that by blending lasing molecules into a carefully chosen host material it is possible to scavenge and deactivate long-lived triplets and so to extend the length of lasing pulses and pulse repetition rate. We investigate organic host materials which show efficient conversion of triplets back into singlet excitons by triplet-triplet annihilation and so can balance STA losses. These results allow us to extend the range of useful sources for optical pumping and to evaluate possible ways towards CW lasing in organic solids.

Acknowledgements
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References
[1] L. Zhang, et al., Materials Horizons, DOI: 10.1039/d5mh01275a (2025).

Revealing and eliminating surface-localized defects for high-performance ambient-processed organic optoelectronics

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The performance of organic optoelectronics is critically limited by charge carrier traps, particularly from the unintentional yet practically unavoidable ambient-induced defects whose origin and distribution are largely unknown; this fundamental gap in understanding impedes the efficiency and scalability of ambient-processed devices. Here, we reveal that the spontaneous defects in ambient-processed organic semiconducting thin films arise from the water-oxygen co-induced doping and packing disorder, and are surface-localized, contrary to the conventional presumption of a uniform bulk distribution. By employing a facile mechanical adhesion method to selectively eliminate those defective surfaces, the power conversion efficiencies (PCEs) of air-processed organic solar cells (OSCs) based on different active layers are boosted to comparable levels of their N2-processed counterparts. Notably, the PCE of D18:L8-BO binary OSC fabricated in air with tape adhesion increases from 17.52% to 19.47%, essentially matching the 19.45~20.05% of their N2-processed counterparts, representing one of the highest PCEs for air-processed OSCs reported to date. Furthermore, the aforementioned strategy enables low-cost ambient-processed interlayer-free OSCs to retain 88.2% of the performance of standard five-layer devices, as well as enhances the detectivity of organic photodetectors, highlighting the effectiveness and universality of eliminating the surface-localized spontaneous defects for high-performance ambient-processed organic optoelectronics.

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References
Revealing and eliminating surface-localized defects for high-performance ambient-processed organic optoelectronics Under Review

Simulating TTM-Based Diradicals: Bridge, Substituent and Vibronic Effects on Excited-State Dynamics

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Tris(2,4,6-trichlorophenyl)methyl (TTM)-based diradicals are promising open-shell systems for molecular spintronics and optoelectronics because of their tunable magnetic coupling and rich excited-state photophysics.(1,2) In this work, we investigate how bridge topology and donor/acceptor substitution modulate the ground- and excited-state electronic structures of TTM-based diradicals. We consider molecules in which two TTM units are connected through different molecular bridges, X-TTM-bridge-TTM-X architectures with electron-donating or electron-accepting substituents (X = D or A), and the limiting case of two TTM units directly linked by a single C-C bond. Ground-state geometries, spin distributions and exchange interactions were characterized using unrestricted DFT from triplet and broken-symmetry singlet configurations. Excited states were described using screened optimally tuned range-separated hybrid functionals with polarizable continuum solvent effects, together with Tamm-Dancoff TD-DFT, spin-flip TD-DFT, mixed-reference spin-flip approaches and multireference CASSCF/QD-NEVPT2 calculations. Spin-orbit couplings and non-adiabatic couplings between excited states were further evaluated, and vibronic effects were included in the calculation of radiative and non-radiative rates. The results show that both the bridging unit and donor/acceptor substitution strongly affect spin distribution, exchange coupling and the nature of low-lying excited states. Natural transition orbital analysis reveals a balance between local excitations and charge-transfer contributions across the diradical framework. These findings clarify structure-property relationships in TTM-based diradicals and provide guidelines for designing open-shell molecular systems with tailored magnetic and photophysical properties.

Acknowledgements
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References

Mesto, D., et al. “Luminescent Trityl-based Diradicaloids: A Theoretical and Experimental Assessment of Charge-Resonance in Low-Lying Excited States.” Chemistry - A European Journal 31, 23 (2025): e202500749.

Abdurahman, A., et al. “A Highly Stable Organic Luminescent Diradical.” Angewandte Chemie International Edition 62, 15 (2023): e202300772.

Skin-Conformal MHz-Speed Organic Photodetectors for Long-Range Near-Infrared Communication

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Near-infrared (NIR) photodetectors are essential components for emerging wearable optoelectronic systems because NIR light offers low biological scattering, reduced ambient interference, and compatibility with free-space optical communication. For skin-integrated platforms, photodetectors must simultaneously provide high bandwidth, low noise, and extreme mechanical deformability. However, ultrathin organic photodetectors (OPDs) typically suffer from a trade-off between mechanical compliance and high-speed operation due to increased series resistance, interfacial recombination, and RC-limited bandwidth under deformation.[1] This work present a 3 μm-thick skin-conformal NIR OPD that achieves MHz-level operation while maintaining stable electrical performance under severe mechanical strain. The device exhibits a specific detectivity of 0.84×10^{14} Jones at 790 nm, extracted from noise-equivalent power measurements, together with a -3 dB cut-off frequency exceeding 1 MHz. Notably, both detectivity and bandwidth are preserved under 66% compressive strain and bending radii below 5 μm. The high-speed and strain-stable characteristics originate from interfacial engineering of a Br-functionalized PACz self-assembled monolayer (SAM). The molecularly thin SAM induces a favorable interfacial dipole that improves energy level alignment and enhances hole extraction while suppressing trap-assisted recombination. This reduces effective series resistance and interfacial capacitance, thereby minimizing RC delay. Transient analysis confirms accelerated photoresponse and suppressed charge accumulation compared to non-functionalized control devices. Importantly, the SAM maintains stable interfacial energetics under strain, enabling MHz-bandwidth photodetection without sacrificing mechanical flexibility.

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References

Youngkyoo Kim, Nature Materials. 5,(2006).

Sungjun Park, Advanced Materials, 30, 34 (2018).

Kangkang Weng, Nature communications, 11,1 (2020)

The Many Roles of Host Materials in Single-Layer Blue OLEDs: Enabling Ohmic Charge Injection, Balanced Transport, and Enhanced Stability

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Blue organic light-emitting diodes (OLEDs) based on thermally activated delayed fluorescence (TADF) emitters still struggle to achieve high operational stability. Single-layer OLEDs, using a single active layer between two electrodes, offer simpler fabrication and improved stability compared with multilayer devices, but matching their efficiency requires barrier-free (Ohmic) charge injection and balanced charge transport. These challenges are particularly severe for blue TADF emitters, whose wide bandgaps hinder injection and electron trapping disrupts charge balance. Here, we show that emitter-host based single-layer architectures can overcome both limitations. Properly selected host materials tune interfacial energetics, enabling efficient injection of both holes and electrons. A simple design rule applies: the host ionization energy (electron affinity) should be at least 0.3 eV higher (lower) than that of the emitter. Using blue TADF emitters DBA-DI and SpiroAc-TRZ, we fabricate single-layer OLEDs achieving external quantum efficiencies (EQEs) above 25%, comparable to state-of-the-art multilayer devices. Electron-transporting hosts such as mCBP-CN further improve charge balance and stability in DBA-DI devices.[1] Optimal emitter concentrations of 20-50% yield EQEs up to 25%. The electron-transporting hosts reduce electron density on DBA-DI, suppressing bond dissociation in its anionic state and enhancing operational stability. The LT_{50} lifetime (1000 cd m^{-2}) increases from 120 hours for neat DBA-DI to 720 hours at 25% DBA-DI. This strategy is general and also applies to carbene-metal-amide (CMA) emitters, a promising class with efficient triplet harvesting and submicrosecond emission lifetimes but limited stability. Optimized CMA:mCBP-CN devices show low turn-on voltage, high power efficiency, minimal roll-off, and sky-blue emission, achieving EQEs above 20% and an LT_{50} of 120 hours at 1000 cd m^{-2}, more than 50x longer than previously reported sky-blue CMA OLEDs.

References

O. Sachnik, N. Kinaret, R. Saxena, M. Manz, W. Liu, J. T. Blaskovits, D. Andrienko, J. J. Michels, P. W. Blom, G.-J. A. Wetzelaer, Nature Materials 24, 1742 (2025).

Thermally activated delayed fluorescence (TADF) in indolizine derivatives: excited-state photophysics under photoexcitation and electroexcitation.

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Thermally activated delayed fluorescence (TADF) has emerged as an efficient strategy for harvesting triplet excitons in purely organic emitters for OLED applications.[1,2] In this work, indolizine was introduced as a new acceptor unit in donor–π–acceptor architectures to explore its potential in TADF materials. Molecular design was guided by DFT and TD-DFT calculations, which provided insights into the distribution of frontier orbitals, the excited-state nature, spin-orbit coupling, and singlet-triplet energy gaps (ΔE_{ST}).

While the parent indolizine (Z) and the carbazole derivative (ZCz) did not show TADF, the phenoxazine- and phenothiazine-based compounds (ZPX and ZPT) exhibited delayed fluorescence. Steady-state and time-resolved photophysical studies in solid-state measurements in PS, PMMA, and mCP matrices demonstrated an efficient triplet harvesting. Temperature-dependent photoluminescence and time-resolved emission spectroscopy indicated the participation of distinct ^{1}LE, ^{3}LE, ^{1}CT, and ^{3}CT states, supporting two delayed fluorescence pathways mediated by reverse intersystem crossing (RISC).

Solution-processed OLEDs with architecture ITO|PEDOT:PSS|mCP:emitter|TPBi|Ca|Al were fabricated using mCP as host. Devices based on ZPX and ZPT achieved external quantum efficiencies of up to 8.7%, close to the calculated theoretical limit of the emitting layer. Comparison of photoluminescence and electroluminescence spectra showed that electrical excitation preferentially populates CT-related states, leading to distinct emission profiles despite the same final emissive state.

These results establish indolizine derivatives as a versatile platform for TADF emitters, covering blue, cyan, green, and yellow emission, and demonstrate the relevance of excitation-dependent excited-state pathways for the design of next-generation optoelectronic materials.

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References

P. L. Dos Santos, M. K. Etherington and A. P. Monkman, Royal Society of Chemistry, 2018, preprint, DOI: 10.1039/c8tc00991k.

E. S. Moraes, J. C. Germino and L. Pereira, Org. Electron., 2025, 137, 107175.

Towards continuous wave organic lasing: A triplet–triplet annihilation upconversion approach to triplet management.

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Despite great efforts, realising continuous wave (CW) lasing in solid-state organic materials continues to be a significant challenge, due to the accumulation of long-lived triplet excitons. These triplets quench radiative singlets via singlet–triplet annihilation (STA). To prevent these losses, triplets must be efficiently removed and deactivated from the organic laser gain material. Here we investigate a triplet recycling approach, which combines triplet scavenging with efficient conversion of these triplets back to singlets by triplet- triplet annihilation (TTA). Not only could this compensate for STA losses, but the regenerated singlets can also contribute to lasing emission. By combining a kinetic rate equation modelling approach, alongside experimental time resolved photo-luminescence measurements [1] of thin films, we show that triplet recycling via TTA presents a potentially promising method of reducing triplet accumulation and losses caused by STA. This work will extend our understanding of the underlying photophysics of these systems which will allow for continued development and eventual realisation of a CW organic laser.

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References
[1] L. Zhang, et al., Materials Horizons, DOI: 10.1039/d5mh01275a (2025).

Ultrafast Structural Dynamics in Luminescence Process in Crystalline Carbazole Benzonitrile Derivatives

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Structural dynamics in the excited states plays a critical role in luminescence process in a molecule: however, it is not often taken into account for understanding the luminescence process. This is because there are few experimental methods with time resolution high enough to track the structural dynamics in the luminescence process. We have been developing various time-resolved measurement methods sensitive to molecular structure and have revealed a variety of photoexcited dynamics in photofunctional materials such as photoactive liquid crystals [1], thermally activated delayed fluorescence (TADF) emitters for OLED [2], and metal complexes for artificial photosynthesis [3]. In this study, we have investigated the excited-state structural dynamics in the picosecond range in carbazole benzonitrile derivatives, 4CzIPN (1,2,3,5-tetrakis(carbazol-9-yl)-4,6-dicyanobenzene) and o-3CzBN (3,4,5-tri(9H-carbazole-9-yl)benzonitrile), in the crystal phase by the combination of structural sensitive methods, time-resolved infrared spectroscopy (TR-IR) and time-resolved electron diffraction (TR-ED), in addition to Kerr-gate time-resolved photoluminescence spectroscopy (TR-PL). Consequently, in 4CzIPN, we found that the structural change upon photoexcitation is restricted except for rotation of one Cz moiety, which leads to quick and non-thermal intersystem crossing (ISC). In o-3CzBN, we found that no intramolecular structural change takes place and the whole molecule is slightly rotated upon photoexcitation, which does not have an influence on the thermal ISC process.

References

[1] M. Hada, S. Saito, S. Tanaka, J. Am. Chem. Soc. 139, 15792 (2017).

[2] M. Saigo, K. Miyata, S. Tanaka, et al. J. Phys. Chem. Lett. 10, 2475 (2019).

[3] Y. Shimoda, K. Miyata, M. Funaki, et al. Inorg. Chem. 60, 7773 (2021).

Understanding the photophysical origin of efficiency roll-off in TADF OLEDs

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We present a new measurement to understand efficiency loss in thermally activated delayed fluorescent (TADF) OLEDs. TADF OLEDs can achieve peak internal quantum efficiencies close to 100%, making them attractive for high-efficiency displays. A major limitation of TADF OLEDs, however, is their efficiency loss at high brightness - an effect known as efficiency roll-off [1].

The photophysics of TADF emitters has been studied extensively in solution and film but such measurements are generally unsuitable for operating TADF OLEDs. This has led to a large degree of uncertainty in identifying the exciton annihilation processes responsible for efficiency roll-off in these devices. In our method based on frequency-domain luminescence, we can easily and quickly resolve emission due to both prompt and delayed photoluminescence (PL) from TADF materials. Our method is also not affected by strong background luminescence signals. This makes it well-suited to understanding exciton annihilation in operating TADF OLEDs and gives it a fundamental advantage over conventional time-resolved PL techniques.

We apply our technique to understand efficiency roll-off in a TADF device based on 15 wt% 1,2,3,5-tetrakis(carbazol-9-yl)-4,6-dicyanobenzene doped 3,3′-di(9H-carbazol-9-yl)-1,1′-biphenyl (15 wt% 4CzIPN doped mCBP). In this device we find that singlet-triplet annihilation (STA) is the dominant process responsible for efficiency roll-off at high currents, followed by singlet-polaron annihilation (SPA), and triplet-polaron annihilation (TPA), and quantify the contribution of each. Following this, we identify the structure-property relations which drive exciton annihilation in TADF materials and propose design improvements which can be applied to minimize efficiency roll-off in TADF OLEDs.

References

Diesing S, Zhang L, Zysman-Colman E, Samuel IDW. A figure of merit for efficiency roll-off in TADF-based organic LEDs. Nature. 2024 Mar 28;627(8005):747–53. doi:10.1038/s41586-024-07149-x

Vacuum-processed organic and perovskite optoelectronics: challenges and opportunities in architecture and device engineering

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Among emerging organic and perovskite optoelectronic devices, our group has focused on the study and evaluation of various systems from a device-architecture perspective, using vacuum thermal evaporation (VTE) as the fabrication method. This scalable, industrially compatible technology enables the fabrication of devices in a reproducible manner, with nanometric control of layer thicknesses and doping, without the limitations of solution methods. In organic photovoltaic devices, we have studied the role of lateral alkyl chains on the molecular ordering of archetypical benzodithiophene units [1], the development of interconnecting systems for tandem devices, and the compatibility of polymeric systems with VTE [2]. In addition, we are exploring the stability of hyperfluorescent organic light-emitting diodes to study degradation mechanisms. In perovskite photovoltaics, using a dual-monitoring configuration, we have achieved high reproducibility for volatile methylammonium-based perovskites. Following this configuration, CsxFA1-xPbI3 has been used to form homojunctions, reducing recombination and increasing charge extraction [3]. Also, the evaluation of lead-free CsSnX3 perovskite has been explored for the fabrication of tandem flexible devices. Finally, perovskite light-emitting diodes have been studied, adjusting their dimensionality to facilitate recombination and enhance device performance and stability.

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References

C. Antoine, D. Vilches, P. Preuss, F. A. Angel, Energy Technology 2024, 12.

A. F. González, P. A. Sobarzo, C. Saldías, C. A. Terraza, F. A. Angel, APL Energy 2025, 3.

F. Barría-Cáceres, F. A. Angel, ACS Applied Energy Materials 2025, 8, 15633.

Zinc Tin Oxide Nanocomposite Deep UV Photodetector Embedded Circuit for Wireless Flame Detection

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Wildfires and large-scale fires require rapid detection at the ignition stage, but conventional technologies often respond slowly or trigger false alarms. Deep ultraviolet (DUV) photodetectors (PD) represent a promising solution. [1, 2] Deep ultraviolet sensing provides a selective approach because solar-blind radiation in the 200–280 nm range originates almost entirely from combustion. We present a flexible and fully integrated DUV flame sensing platform based on a zinc tin oxide (ZTO) nanocomposite photodetector directly fabricated on a wireless flexible circuit. The system incorporates amplification, power management, and Bluetooth communication for standalone monitoring (Figure 1). A uniform 65 nm ZTO nanocomposite layer with a 3.97 eV bandgap enables strong solar-blind selectivity. The device architecture (ITO/ZTO/CuSCN/PEDOT:PSS) shows negligible response under ambient light and a rapid photocurrent upon 265 nm irradiation (Figure 2). Flame-sensing tests with a torch, solid fuel, and gas stove at 20 cm demonstrated clear and distinct signal changes of approximately 23 percent, 59 percent, and 97.8 percent, respectively, without false alarms under sunlight or indoor lighting (Figure 3). Time-dependent features extracted from these responses were used to train machine learning models that successfully classified flame types and estimated relative distance. In summary, this ZTO-based solar-blind DUV platform provides a thin, flexible, low-power sensing solution capable of wireless operation and flame classification. The system offers a practical foundation for distributed and autonomous early-warning networks for wildfire and large-scale fire detection.

References

Ma, Jingli, et al., Advanced Functional Materials, 35.10, 2414943 (2025).

Zou, Bocong, et al. Advanced Functional Materials, 35.15, 2421819 (2025).

A Pyridine-3,5-dicarbonitrile Emitter with Polymorphism-Dependent Luminescence and Efficient OLED Performance

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Donor–acceptor organic emitters, particularly pyridine-3,5-dicarbonitrile derivatives, have been widely explored as thermally activated delayed fluorescence (TADF) materials for OLED applications due to their tunable electronic structure [1, 2]. In this work, we report on the synthesis and characterization of six new pyridine-3,5-dicarbonitrile derivatives, designed to investigate the relationship between molecular structure, solid-state organization, and emission properties. Photophysical studies revealed distinct behaviors across the series. Among the compounds, PXZ-tPPC exhibited remarkable polymorphism-dependent emission, with different luminescent responses associated with its crystalline forms. In addition, this compound showed pressure-dependent emission, demonstrating the sensitivity of its excited states to changes in molecular packing and external stimuli. These results highlight the role of solid-state organization in modulating emission processes in TADF systems. Based on its promising properties, PXZ-tPPC was preliminarily evaluated as the emissive layer in an OLED device with the architecture ITO/Molybdenum trioxide(MoO3) (8nm)/ 4,4'-(cyclohexane-1,1-diyl)bis(N,N-di-p-tolylaniline) (TAPC) (50nm)/1,3-carbazol-benzene (mCP) (10nm)/N,N-Dicarbazolyl-4,4'-biphenyl (CBP) : 10wt% PXZ-tPPC (20nm)/4,7-diphenyl-1,10-phenantroline (Bphen) (45nm)/Lithium floride (LiF)/Aluminum (Al) (70nm), reaching a maximum external quantum efficiency (EQE) of 12% and luminance up to 19,000 cd m^{-2}. These results demonstrate the potential of PXZ-tPPC as an efficient emitter and provide further insight into how polymorphism and external stimuli influence emission in pyridine-3,5-dicarbonitrile-based systems.

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References

J. M. Dos Santos et al., Chem. Rev., 124, 13736–14110 (2024).

Z. Chen et al., J. Mater. Chem. C, 6, 6543–6548 (2018).

Correlated 1/f³ Noise in Photo-NDR DNTT/TiO2 Heterojunctions for Secure Bio-signal

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Noise is an inherent characteristic of all semiconductor devices; however, its interpretation and significance vary depending on the analytical context. Historically, low-frequency noise (LFN) spectroscopy has been utilized as a nondestructive diagnostic technique to probe deep-level defects, interfacial irregularities, and charge transport mechanisms in electronic systems. Despite its diagnostic utility, the associated current fluctuations have conventionally been viewed as undesirable artifacts that degrade circuit performance and thus necessitate suppression. In recent years, this perspective has evolved: LFN is increasingly recognized as a viable on-chip entropy source for emerging stochastic electronics, whereby intrinsic fluctuations are no longer merely limitations, but functional resources that can be strategically harnessed. Building upon this emerging paradigm, We report the first observation of correlated 1/f³ LFN in a photo-induced negative differential resistance (NDR) device based on a DNTT/TiOx heterojunction. This unusual noise behavior arises from the correlation between carrier generation-recombination and trapping/detrapping processes at the organic/inorganic interface, as revealed by systematic bias- and illumination-dependent noise analysis. The presence of distinct noise signatures across different voltage regimes provides critical insight into the NDR mechanism, characterized by a transition from band-to-band tunneling to diffusion-dominated transport under photoexcitation. Furthermore, we demonstrate that the unique tunability of noise characteristics by light and voltage enables multiple applications within a single device: (i) extraction of PPG signals followed by noise-based encryption, (ii) NDR-enabled signal inversion, and (iii) low-noise image readout.

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References

Lee, Gyeongho, et al. "Heterostructure of Reduced Titanium Dioxide Nanorods and Small Molecules Leads to Photo-Induced Negative Differential Resistance Behaviors." Advanced Optical Materials 12.15 (2024): 2303050.

Delocalisation enables efficient inter-chain exciton separation in conjugated polymers

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Understanding how interactions between molecular chains control the efficiency of exciton separation and charge generation is critical for improving the performance of organic solar cells. Efficient and fast, sub-100 fs charge generation in polymer-based bulk heterojunction devices has been attributed to interchain exciton delocalisation [1]. However, accurately modelling exciton separation in these materials is difficult, as it requires tracking the correlated motion of two charges that can quantum-mechanically delocalise within and across molecular chains. This challenge is compounded by polaron formation, due to the coupling of electronic states to environmental vibrations, and by electronic disorder, neither of which are necessarily small enough to permit standard perturbative treatments. To address these challenges, we employ the secular polaron-transformed Redfield equation (sPTRE) [2] to model the complete photophysical pathway from optical absorption to charge generation for isolated chains and multi-chain assemblies. The sPTRE accurately models charge generation over a wide range of coupling and disorder strengths by transforming the charge-generation problem into a frame where the system-environment coupling is weak, allowing an accurate treatment within perturbative Redfield theory [2]. Using the sPTRE, we demonstrate how interchain exciton delocalisation enables efficient charge generation via interchain charge-transfer states. Finally, we investigate the impact of chain packing, relative orientation, chemical structure, and conformation on the efficiency of charge generation by combining our computational approach with quantum-chemical calculations and structural motifs from coarse-grained molecular dynamics.

References

Z. Guo, et al, J. Am. Chem. Soc., 136, 28 (2014)

C. K. Lee, et al, J. Chem. Phys., 142, 164103 (2015)

Development of a TiO2-Nb- Based anodic Electrode for Enhanced Photovoltaic Conversion Efficiency in DSSCs

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The development of doped semiconductor photoanodes has been widely investigated as an effective strategy to improve charge transport and photovoltaic performance in dye-sensitized solar cells (DSSCs). Among the possible dopants, niobium is known to function as an electron donor in TiO_2, contributing to increased electrical conductivity and improved electron mobility within the semiconductor matrix. In this work, Nb-doped TiO_2 thin films were fabricated on fluorine-doped tin oxide (FTO) substrates by spin coating. Three compositions were investigated: 1%, 2%, and 4% Nb relative to TiO_2. After deposition, the films were thermally treated at 450 °C to promote crystallization and improve structural organization. The morphology and structural properties of the films were characterized by atomic force microscopy (AFM) and Fourier transform infrared spectroscopy (FTIR). AFM analysis revealed homogeneous nanostructured surfaces for all compositions, with a granular distribution of nanostructures over areas of 50 µm × 50 µm. Among the investigated samples, the electrode containing 2% Nb exhibited the most uniform morphology and the highest density of nanostructures, indicating a larger effective surface area that may favor dye adsorption in DSSC photoanodes. In contrast, the films containing 1% and 4% Nb showed lower nanograin density and greater surface heterogeneity. FTIR spectra confirmed the characteristic TiO2 vibrational bands in the 800–1000 cm^{-1} region and the presence of surface hydroxyl groups around 3400 cm^{-1}. The sample with 2% Nb showed stronger TiO2 related bands, suggesting improved structural organization and possible substitutional incorporation of Nb into the TiO_2 lattice. These results indicate that Nb doping, particularly at 2%, significantly influences the surface morphology and structural properties of TiO_2 films have strong potential for improving charge transport and overall photovoltaic performance in DSSC devices.

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References

O'Regan, B., Grätzel, M, Nature, 353, 737-740, (1991)

H. O. Cunha, A. M. B. Leite, Colorants, 3, 329-349 (2024)

A. M. B. Leite, et al., Colorants, 3, 307 (2024)

Dual-Chromophore Isolation Strategies for Efficient Upconversion in TADF Emitters via Rigid, Covalent Bridges

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The development of high-efficiency organic light-emitting diodes (OLEDs) hinges on the precise control of excited-state dynamics in thermally activated delayed fluorescence (TADF) emitters. A promising approach involves the use of dual-chromophore architectures, in which multiple chromophores are integrated into a single emitter molecule. The degree of conjugation between these chromophores inherently governs the emitter's optical and electronic properties, with recent studies indicating that a reduction in conjugation enhances device performance. In this study, we investigate a dual-chromophore TADF emitter linked by a series of rigid, covalent bridges. These bridges systematically modulate the degree of conjugation and through-space coupling, significantly influencing key photophysical properties, including the singlet-triplet gap and the associated emission pathways available. Our findings demonstrate that sterically hindered and electronically decoupling bridges effectively reduce conjugation, leading to distinct emission profiles, and ultimately aiming to enhance exciton utilisation and improve device efficiency. This work offers a rational framework for the next generation of OLED devices, emphasising the pivotal role of bridge-mediated tuning of TADF emitters for optimised performance and efficiency.

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References
Cho, Y.J., Jeon, S.K., Chin, B.D., Yu, E. and Lee, J.Y. (2015). The Design of Dual Emitting Cores for Green Thermally Activated Delayed Fluorescent Materials. Angewandte Chemie International Edition, 54(17), pp.5201–5204. doi:https://doi.org/10.1002/anie.201412107.

Effect of composition on thermally evaporated $CsPbBr_3$–Cs_4PbBr_6 thin films to promote radiative recombination in efficient and stable optoelectronic devices

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The compositional transition between the inorganic perovskite phases $CsPbBr_3$ (3D) and Cs_4PbBr_6 (0D) leads to significant changes in the crystal structure, Pb–Br–Pb connectivity, and the dimensionality of the octahedral units, all of which directly influence the optical properties of the material. In this work, thin films were fabricated by thermal evaporation, a deposition technique that enables precise control of the deposition rate throughout the synthesis process, in contrast to solution-based methods where such control is often more limited. Using this approach, we investigate the structural and photoluminescence evolution of the films by correlating the CsBr:$PbBr_2$ ratio with the preferential formation of 3D and 0D domains. The progressive incorporation of the Cs_4PbBr_6 phase promotes enhanced electronic localization, energy-level shifts, and variations in photoluminescence intensity. These effects are attributed to changes in surface passivation, defect density, and octahedral connectivity. This analysis is supported by advanced optical characterization, which reveals how radiative and non-radiative recombination processes depend on composition and the local chemical environment. Based on the optical and structural characterizations, we demonstrate that compositional optimization enhances photoluminescence and enables the study of degradation mechanisms associated with surface defects and ionic instability, two critical factors for the development of low-power lighting technologies. Furthermore, compositional tuning promotes radiative recombination pathways in optoelectronic devices, thereby improving the emission efficiency of the material. A deeper understanding of the interplay between structure, photophysics, and stability in these hybrid perovskites provides a clear pathway toward the design of more efficient PeLEDs suitable for energy-stable lighting applications.

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References

Du, P.; Wang, L.; Li, J.; Luo, J.; Ma, Y.; Tang, J.; Zhai, T. Thermal Evaporation for Halide Perovskite Optoelectronics: Fundamentals, Progress, and Outlook. Advanced Optical Materials. John Wiley and Sons Inc February 1, 2022. https://doi.org/10.1002/adom.202101770

Bae, S. R.; Seol, M. J.; Kim, S. Y. CsPbBr3 and Cs4PbBr6 Perovskite Light-Emitting Diodes Using a Thermally Evaporated Host-Dopant System. Nanoscale 2023, 15 (21), 9533–9542.

https://doi.org/10.1039/d3nr01190a.

Bai, T.; Wang, S.; Zhang, K.; Chu, C.; Sun, Y.; Yi, L. High Stability and Strong Luminescence CsPbBr3-Cs4PbBr6 Thin Films for All-Inorganic Perovskite Light-Emitting Diodes. RSC Adv 2023, 13 (35), 24413–24422. https://doi.org/10.1039/d3ra03947a.

Environmental Stability of Carbazole-based Self-Assembled Monolayers in Organic Solar Cells under the ISOS-O-2 Outdoor protocol

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Organic solar cells (OSCs) have recently exceeded 20% energy conversion efficiency (PCE); however, long-term operational stability remains a major bottleneck for industrial application. Conventional hole transport layers (HTLs), such as PEDOT:PSS, are known to limit device lifetime due to their acidic and hygroscopic nature [1]. In contrast, carbazole-based self-assembled monolayers (SAMs), such as Br-2PACz, have emerged as promising ultrathin alternatives, improving energy level alignment, passivating interfacial defects and enhancing device performance [2]. Despite these advantages, the structural integrity and dipole alignment of such SAMs under real-world operating conditions remain poorly understood. This work, therefore, investigates the stability of SAM-based OSCs under the ISOS-O-2 (Outdoor, intermediate) protocols [3], which reproduces the combined effects of natural solar irradiance, ambient humidity and temperature fluctuations. Devices were fabricated using three HTL architectures: (i) conventional PEDOT:PSS, (ii) a Br-2PACz self-assembled monolayer, and (iii) a dual-layer Br-2PACz/PEDOT:PSS configuration. Device degradation was monitored through the T80 lifetime parameter under outdoor exposure. Our results demonstrate that Br-2PACz devices exhibit faster degradation compared with PEDOT:PSS. Remarkably, the dual-layer Br-2PACz/PEDOT:PSS architecture significantly outperforms both individual HTLs, maintaining superior interfacial stability and a higher Fill Factor (FF) over extended outdoor exposure. By combining the favorable energy level alignment of SAM with the protective properties of the polymer matrix, this work demonstrates a strategic path toward achieving the T80 benchmarks required for commercialization of organic photovoltaic panels.

Acknowledgements
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References

Y. Tong, B. Xu, and F. Ye, Adv. Funct. Mater., vol. 34, no. 10, p. 2310865, 2024.

M. Li, et al, Chemical Review., vol. 124, no. 5, pp. 2138–2204, 2024.

M. O. Reese et al., Solar Energy Materials and Solar Cells, vol. 95, no. 5, pp. 1253–1267, 2011.

From Molecular Structure to Device Stability: BDT and BODIPY-Based Materials for OPV and OLED Applications

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This work presents a comprehensive study on the stability, optoelectronic properties, and device performance of organic semiconductor materials based on benzo[1,2-b:4,5-b']dithiophene (BDT) and 4,4'-difluoro-4-bora-3a,4a-diaza-s-indacene (BODIPY), with applications in both organic photovoltaic (OPV) and organic light-emitting diode (OLED) devices. The physicochemical properties of the materials were characterized prior to the evaporation of the active layers, including optical, electrochemical, and thermal analyses. These properties were correlated with the performance of devices fabricated via vacuum-deposited architectures. OPV devices were fabricated using a bulk heterojunction architecture: ITO|MoO3|X:C60|Bphen|Liq|Al (X = BDT, BODIPY) and evaluated through current–voltage (J–V) measurements and external quantum efficiency (EQE) [1]. In parallel, OLED devices were fabricated by thermal evaporation using the architecture: ITO|MoO3|NPB|X|Alq3|Bphen|Liq|Al (X = BDT, BODIPY) and evaluated through electroluminescence and quantum efficiency measurements [2]. To complement the experimental results, density functional theory (DFT) calculations were performed, including relaxed potential energy surface (PES) scans of key bonds, together with natural bond orbital (NBO) analysis. These calculations offer detailed insight into molecular stability, bond strength, and the electronic and structural factors governing degradation mechanisms [3]. Stability studies were conducted under controlled conditions specific to each type of device. In OPV devices, degradation was evaluated through selective irradiation using different wavelength ranges. In OLED devices, stability was investigated under varying current densities to assess their impact on operational stability.

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References

J.J. Chen, S.M. Conron, P. Erwin, M. Dimitriou, K. McAlahney, M.E. Thompson, High-Efficiency BODIPY-Based Organic Photovoltaics, ACS Appl. Mater. Interfaces. 7 (2015) 662–669. https://doi.org/10.1021/am506874k.

M. Chapran, E. Angioni, N.J. Findlay, B. Breig, V. Cherpak, P. Stakhira, T. Tuttle, D. Volyniuk, J. V. Grazulevicius, Y.A. Nastishin, O.D. Lavrentovich, P.J. Skabara, An Ambipolar BODIPY Derivative for a White Exciplex OLED and Cholesteric Liquid Crystal Laser toward Multifunctional Devices, ACS Appl. Mater. Interfaces. 9 (2017) 4750–4757. https://doi.org/10.1021/acsami.6b13689.

S.-C. Dong, L. Xu, C.W. Tang, Chemical degradation mechanism of TAPC as hole transport layer in blue phosphorescent OLED, Org. Electron. 42 (2017) 379–386. https://doi.org/10.1016/j.orgel.2016.11.041.

From Solution to Device: Aggregation-Induced Enhanced Emission and twisted intramolecular charge transfer in a Pyridylcarbodinitrile for tunable Photoluminescence and OLED applications

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The development of organic luminophores with tunable photophysical properties is crucial for advancing high-performance optoelectronic devices. In this work, a series of phenylpyridylcarbodinitrile (PPC) derivatives with donor–π–acceptor (D–π–A) architectures were synthesized via a Hantzsch multicomponent reaction followed by Suzuki cross-coupling, aiming to correlate molecular structure with solvent-, aggregation-, and device-dependent emission behavior. Four PPC derivatives bearing distinct donor groups were evaluated: 2M-PPC, BP-PPC, FL-PPC, and MT-PPC.

Among them, MT-PPC exhibited remarkable photophysical versatility, characterized by pronounced solvatochromism with an emission shift of 118 nm, indicative of twisted intramolecular charge transfer (TICT) states [1]. Additionally, MT-PPC showed aggregation-induced enhanced emission (AIEE), with a nineteenfold increase in photoluminescence quantum yield upon aggregation. Thin films incorporating MT-PPC in a spiro-phosphine oxide (SF3PO) host matrix displayed tunable emission as a function of dopant concentration, with lower concentrations leading to blue-shifted photoluminescence due to the solid-state solvation (SSS) effect [2].

Organic light-emitting diode (OLED) devices were fabricated with the multilayer structure: ITO / MoO3 / TAPC / TCTA / mCP / SF3PO:MT-PPC (5–20%) / 3TPyMB / LiF / Al. The layers were deposited by thermal evaporation under high vacuum (~10^{-4} Pa) in a glovebox-integrated system. The OLEDs demonstrated concentration-dependent electroluminescence, with emission maxima ranging from 438 to 460 nm and CIE coordinates from (0.18, 0.15) to (0.20, 0.26). The device with 20% MT-PPC achieved a maximum luminance of 977 cd·m^{-2} and an external quantum efficiency (EQE) of 0.80%. These results highlight MT-PPC as a multifunctional luminophore with emission tunability in solution, films, and devices, reinforcing its potential for sensors and optoelectronic technologies [3].

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References

Grabowski, Z. R., et al. (2003). Chemical Reviews, 103(10), 3899-4032

Bulović, V., et al. (1999). Chemical Physics Letters, 308(3-4), 317-322

Vesga-Hernández, C., et al. (2025). Journal of Photochemistry & Photobiology, A: Chemistry, 464, 116312

Functional Organic Materials for Sustainable Photonics: Room-Temperature Phosphorescence - Matrix Effects Tunnelling Phosphorescence Lifetime

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Purely organic materials exhibiting room-temperature phosphorescence (RTP) attract strong interest because they combine persistent emission with the prospect of harvesting up to 100% of electrically generated excited states, while remaining potentially low-cost and highly solution-processable. These attributes position RTP materials for applications in security/anti-counterfeiting, sensing, bioimaging, and optoelectronic devices [1][2]. Nevertheless, establishing reproducible design rules that explain how molecular structure and host microenvironment cooperate to stabilize triplet states and suppress loss pathways under ambient conditions remains challenging. This work investigates the molecules KSH06-71 and KSH06-79, which display RTP in dispersed systems, enabling correlations among matrix-dependent variations in emission intensity, quantum efficiency, and lifetime [3]. A central element is the involvement of n–π* states associated with heteroatoms (N–O), which enhance intersystem crossing (ISC) and promote triplet population; however, long-lived RTP requires effective suppression of nonradiative deactivation (knr). In this context, hydrogen bonding plays a key role by inducing local rigidification, restricting conformational and vibrational motions, reducing internal relaxation, and thereby mitigating nonradiative pathways. The emitters are dispersed in PMMA, Zeonex, and PAA matrices that differ in rigidity, polarity, O_2 permeability, and their ability to form distinct hydrogen-bond networks. In PAA, a stronger hydrogen-bond network increases emitter confinement and, combined with low oxygen permeability, sustains RTP with visible afterglow exceeding 8 s. Characterization employs absorption spectroscopy and steady-state and time-resolved photoluminescence, quantifying yields, lifetimes, and spectral signatures to build a mechanistic picture of RTP in purely organic films.

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References

ZHANG, Xue et al. A class of organic units featuring matrix-controlled color-tunable ultralong organic room temperature phosphorescence. Advanced Science, v. 10, n. 3, p. 2206482, 2023

HE, Tongyu et al. Multi-colour room-temperature phosphorescence from fused-ring compounds for dynamic anti-counterfeiting applications. Chemical Communications, v. 60,

n. 30, p. 4060-4063, 2024

KWON, Min Sang et al. Tailoring intermolecular interactions for efficient room-temperature phosphorescence from purely organic materials in amorphous polymer matrices. Angewandte Chemie, v. 126, n. 42, p. 11359-11363, 2014.

Heteroleptic Copper(I) and Silver(I) Complexes for Light-Emitting Devices

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Sustainable solid-state lighting (SSL) technologies, such as OLEDs and LEECs, are key to addressing global energy demands. Copper(I) complexes represent attractive alternatives to noble metal emitters due to their low cost, abundance, and reduced toxicity. Here, two series of heteroleptic complexes, [Cu(Me-dpa)(Xantphos)]BF_4 (Cu1–2) and [Ag(Me-dpa)(Xantphos)]BF_4 (Ag1–2), were synthesized and evaluated as LEEC.
The complexes were characterized by multinuclear NMR and cyclic voltammetry, and their photophysical properties were studied by UV–Vis and emission spectroscopy in solution and solid state. LEEC devices were fabricated using Cu1 and Cu2 (ITO/PEDOT:PSS/emissive layer/Al).
In solution, both series exhibit emission around 350 nm with oxygen sensitivity, suggesting triplet-state involvement. In the solid state, strong photoluminescence was observed: green emission for Cu(I) and blue for Ag(I). Asymmetric complexes (Cu2 and Ag2) show dual emission, indicating multiple emissive states.
Cu(I)-based LEECs were operational, whereas Ag(I) analogues were unstable. Cu1 showed stable emission, while Cu2 exhibited voltage-dependent electroluminescence (see Figure 1). These results highlight the potential of Cu(I) complexes for light emitting devices, with ongoing efforts to improve efficiency and stability.

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References
[1] O. Moudam, et al., RCS Advances, 5, 95047 (2015).

[2] A. Villegas-Menares, et al., Dalton Transactions, 54.18, 7306 (2025).

Higher-Order Harmonics Probed by Nonlinear Impedance Spectroscopy in Perovskite Solar Cells Based on Niobium MXenes

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Perovskite solar cells (PSCs) are promising photovoltaic devices due to their excellent optoelectronic properties. To better understand metastability and aging, advanced materials and improved electrical characterization techniques have been introduced to enhance stability. In this work, we evaluate the effect of two-dimensional niobium-based materials, including Nb MAX phases and Nb MXenes, on PSC performance, stability, and harmonic response. These materials exhibit outstanding electrical and chemical properties, improving interfacial quality and acting as protective barriers. Devices were fabricated in a controlled glovebox environment with an n–i–p architecture, reaching a power conversion efficiency of 17.5%. Dynamic processes were investigated using conventional Impedance Spectroscopy (IS) and Nonlinear Electrical Impedance Spectroscopy (NLEIS) over a frequency range from 1 Hz to 10 MHz. IS provides insight into charge transport and recombination, while NLEIS analyzes higher-order harmonic responses under large perturbations. The evaluation of second and higher-order harmonics reveals nonlinear effects related to ion migration, field-dependent recombination, interfacial charge accumulation, and carrier extraction. Complementary cyclic voltammetry under illumination correlates current–voltage behavior with nonlinear impedance features. PSCs are sensitive to external electric fields, which promote ionic redistribution and reversible performance changes, while environmental aging causes irreversible degradation. The incorporation of Nb-based materials improves interfacial stability and charge extraction. Harmonic analysis through NLEIS enhances sensitivity to interfacial and bulk processes, providing deeper understanding of degradation mechanisms and guiding strategies to improve efficiency and long-term stability.

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References

V. Lopez-Richard, et al., Physical Review B, 110, 115306 (2024).

S. Paramadam, et al., ACS Applied Energy Materials, 8, 9049 (2025).

G. L. Nogueira, et al., Solar RRL, 9, e202500562 (2025).

Hole Trap Formation in Quantum Dot Light-Emitting Diodes Under Electrical Stress

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Quantum dot light-emitting diodes (QLEDs) have emerged as promising candidates for next-generation display technology, but the limited lifetime of QLEDs hampers their further commercialization. Despite extensive research that has been conducted for the last decades, the mechanism leading to the rapid degradation of QLEDs remains unclear. Here, charge transport in blue Cd-based quantum dots (QDs) exhibits thermally activated hopping of holes with an activation energy of 0.30 eV, well described by the extended Gaussian disorder model. In blue QLEDs, transient electroluminescence reveals that charge transport in pristine devices is dominated by hole transport in the QD layer. During degradation, hole transport decreased due to hole trap formation. Impedance measurements show enhanced negative capacitance in degraded devices, directly evidencing hole trap formation. These traps introduce additional trap-assisted recombination between trapped holes and free electrons, as confirmed by electroluminescence spectra evolution, leading to efficiency loss. Numerical simulations quantify the hole trap density as a function of aging time, which matches impedance spectroscopy results, validating hole trap formation as the key degradation mechanism in QLEDs.

References

S. Li, P. W. M. Blom and Q. Niu, Advanced Electronic Materials, 10, 2400142 (2024).

W. Lin, P. W. M. Blom and Q. Niu, Journal of Applied Physics, 135, 045701 (2024).

J. Huang, P. W. M. Blom and Q. Niu, Advanced Electronic Materials, 11, 2400231 (2025).

HS- OLEDs using indolocarbazole-based emitters with balanced charge transport and enhanced solid-state emission

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Following the initial demonstrations of electroluminescence in simple OLEDs, substantial efficiency improvements were achieved by introducing multiple functional layers and by harvesting triplet excitons. In addition, recent advances in simplified device architectures, based on a single material with balanced charge transport or partial doping, have matched or even surpassed the performance of complex multilayer OLEDs [1], while also significantly reducing the environmental footprint of the devices. Herein, low molecular weight emissive compounds were developed by functionalizing an indolocarbazole core with fluorenyl and tetraphenylethenyl (TPE) moieties. The designed compounds were synthesized and thoroughly characterized using a combination of theoretical calculations and experimental techniques. Indolocarbazole core offers a unique combination of strong hole-donating ability, high thermal and triplet-energy stability, tunable electronic properties, and excellent film-forming behavior, making them highly attractive for OLED and organic electronic applications. The fluorenyl unit was introduced to balance charge carrier mobilities, while the incorporation of TPE fragment enhances the photophysical properties in the solid state. The thermal, electrochemical, and photophysical properties of the synthesized compounds were studied. In addition, simple-architecture OLEDs employing these materials in different active layers were fabricated and evaluated reaching EQEmax=4.95%.

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References
O. Sachnik, et al., Advanced Materials, 35, 2300574 (2023)

Hyperfluorescent Host-Free OLEDs for Organic Upconversion Devices

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Efficient detection and imaging in the near-infrared (NIR) spectral region are critical for applications ranging from information technologies to robotics and machine vision. While current technologies rely on inorganic semiconductors, all-organic upconversion devices (OUDs) have emerged as promising alternatives. OUDs consist of a monolithic integration of an organic NIR photodetector and an organic light-emitting diode (OLED), enabling wavelength upconversion within a fully organic platform [1,2].

In this work, we report host-free hyperfluorescent (HF) OLEDs designed for OUD architectures. The devices employ CzDBA (5,10-Bis(4-(9H-carbazol-9-yl)-2,6-dimethylphenyl)-5,10-dihydroboranthrene) as a thermally activated delayed fluorescent (TADF) sensitizer and a fully evaporated indole squaraine (ISQ) dye (1,3-Bis[(3,3-dimethylindolin-2-ylidene)methyl] squaraine) as the final fluorescent emitter. Squaraine dyes are attractive due to their narrowband red/NIR emission and high photophysical stability. In parallel, the fluorescent dye DCM2 is considered an alternative emitter, as its emission presents a stronger spectral overlap with CzDBA, potentially enabling more efficient Förster resonance energy transfer (FRET).

Emitting layers were fabricated via thermal co-evaporation of CzDBA and ISQ (0–10 wt%). The OLED structure consists of MoO_3/C_{60}/CzDBA:ISQ/TPBi/Al. CzDBA-only OLEDs exhibited high luminance up to 170,000 cd·m^{-2} (560 nm). Upon incorporation of ISQ, energy transfer from the TADF sensitizer to the squaraine emitter was achieved, resulting in a pronounced spectral shift toward 670 nm with a narrowed emission bandwidth.

These results demonstrate the successful realization of a two-component, host-free HF-OLED architecture and highlight the potential of squaraine-based and alternative fluorescent emitters for high-performance organic upconversion and NIR optoelectronic devices.

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References

W.-H. Hu, J. P. F. Assunção, R. dos S. Carvalho, E. Didier, M. Diethelm, S. Jenatsch, D. Bachmann, I. Shorubalko, M. Cremona, F. Nüesch, M. Bauer, R. Hany, Photomultiplication Enabling Efficient Shortwave Infrared-Sensitive Organic Upconversion Devices. Adv. Funct. Mater. 2024, 34, 2407528. https://doi.org/10.1002/adfm.202407528

W.-H. Hu, C. Vael, M. Diethelm, K. Strassel, S. B. Anantharaman, A. Aribia, M. Cremona, S. Jenatsch, F. Nüesch, R. Hany, On the Response Speed of Narrowband Organic Optical Upconversion Devices. Adv. Optical Mater. 2022, 10, 2200695. https://doi.org/10.1002/adom.202200695

Kotadiya, N.B., Blom, P.W.M. & Wetzelaer, GJ.A.H. Efficient and stable single-layer organic light-emitting diodes based on thermally activated delayed fluorescence. Nat. Photonics 13, 765–769 (2019). https://doi.org/10.1038/s41566-019-0488-1

Interfacial Modulation in Hybrid Emitters Based on Rare-Earth Doped TiO_2 and D-π-A Quinoline Derivatives

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Hybrid organic–inorganic heterostructures offer a promising design for devices by combining the high luminescence efficiency of organic semiconductors with the chemical stability and charge transport capability of metal oxides[1]. In this work, TiO2 thin films doped with Er3+ and Yb3+ are coupled to a D-π-A quinoline derivative forming hybrid heterostructures. Structural analysis confirmed preservation of TiO2 anatase phase after doping, with slight modifications in preferential orientation and surface morphology. Optical absorption revealed characteristic intra-4f transitions of the lanthanides, indicating the introduction of localized states within the TiO2 bandgap. FTIR spectroscopy revealed clear evidence of interfacial chemical interaction through deprotonation of the quinoline carboxylic group and coordination to surface Ti sites. For Er3+ a well-defined bridging bidentate configuration was identified, indicating strong and organized anchoring of the organic layer. In contrast, Yb3+ exhibited a less defined coordination environment, suggesting a more heterogeneous interface. Photoluminescence measurements showed a blue shift from 500 to 483 nm upon heterostructure formation, evidencing modification of the excited-state electronic structure due to interfacial coupling[2]. Electroluminescence data exhibit diode-like behavior for all doped systems. The Er3+ heterostructure exhibited a lower turn-on voltage (5 V), associated with stronger interfacial coupling and facilitated charge injection, whereas Yb3+ devices required higher bias but showed improved emission stability under higher electric fields. These results demonstrate that rare-earth doping actively modulates interfacial coordination strength, which in turn governs excited-state dynamics.

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References

Zhou, K., Qi, B., Liu, Z., Wang, X., Sun, Y., Zhang, L. Adv. Funct. Mater., 2024, 34, 2411671.

Zhang, Q., Li, M., Li, L., Geng, D., Chen, W., Hu, W. Chem. Soc. Rev., 2024, 53(6), 3096-3133.

Ion Migration and Hysteresis in Perovskite Solar Cells: Insights from Capacitance-Frequency Analysis

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Ion migration is a key phenomenon that influences the performance and stability of metal halide perovskite solar cells (PSCs). Mobile species such as halide ions and organic cations migrate by hopping between vacant lattice sites under internal or applied electric fields, leading to redistribution of ionic charge within the material. This leads to current–voltage (J–V) hysteresis, as ions respond more slowly than electronic carriers, causing nonequilibrium behavior during measurements. The accumulation of ions at interfaces or within the bulk affects the electrical potential landscape, which influences charge extraction, recombination[1], and overall efficiency. This typically leads to time-dependent performance and challenges in accurate characterization.

Capacitance frequency (C–f) analysis provides a powerful, non-destructive way to probe these ionic effects by separating slow ionic responses from fast electronic processes. At low frequencies, capacitance is dominated by ion accumulation and interfacial polarization, whereas at high frequencies it mainly reflects electronic charge dynamics. This frequency-dependent response enables the extraction of key parameters such as ion mobility and ion density, ion mobility primarily determines the scan-rate regime at which hysteresis becomes pronounced, while ion density governs the magnitude of the hysteresis[2]. Since hysteresis in PSCs originates from the coupling between ionic motion and electronic transport, it leads to transient behavior and performance variation over time. A comprehensive understanding of ion-induced hysteresis, supported by techniques like C–f analysis, is essential for improving the accuracy of device characterization and for designing stable, high-performance perovskite solar cells suitable for practical applications.

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References

O. Sandberg, M. Kumar, M. Stolterfoht, M. Nyman, D. Neher, & A. Armin “Analytical model for interface recombination limited ideality factors in p -i -n perovskite solar cells” APL Energy 3, 036107 (2025)

M. Kumar, C. Ding, J. Yang, O. Sandberg, M. Nyman, C. Ma, & R. Österbacka “Effect of thermal stress on the ion density and mobility distribution in perovskite solar cells” Journal of Physical Chemistry Letters, 17(5), 1527–1533 (2026)

Nanostructures for efficient organic light-emitting diode emission management

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OLEDs are increasingly applied in illumination and displays because they offer excellent color quality, are mechanically flexible, and are self-emissive. Their usage is, however, limited by their low external quantum efficiency and efficiency roll-off at high driving voltages. This, together with demands for smaller pixels and device sizes in emerging technologies, motivates innovations that increase efficiency and allow replacing external optical elements used for light manipulation with embedded solutions. Commonly, the research towards outcoupling enhancement in OLEDs focuses on molecular design of the emitters and on various external components, such as Micro Lens Arrays and substrate roughening [1,2]. External components can only be used to extract substrate modes, are often bulky, and expensive to manufacture. Here, we demonstrate enhanced outcoupling as well as directional and polarization control of emission with the inclusion of nanostructures within OLED devices. Unlike the external solutions, the inclusion of nanostructures allows extraction of light from all lossy modes. Furthermore, they are compatible with miniturization demands of the devices. We have realized maximum enhancement of 30% at near-normal directions as well as significant narrowing and blue-shifting of the emission profile. Furthermore, non-trivial nanostructures, that provide angle-independent color of emission, have been studied and shown promise. Lastly, polarization dependent response with a degree of linear polarization, defined via Stokes parameters as S1/S0, has been observed with a ration of 0.3 at the strongest modes.

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References
[1] Möller, S.; Forrest, S. R. Improved Light Out-Coupling in Organic Light Emitting Diodes Employing Ordered Microlens Arrays. Journal of Applied Physics 2002, 91, 3324–3327

[2] Zhou, J.; Ai, N.; Wang, L.; Zheng, H.; Luo, C.; Jiang, Z.; Yu, S.; Cao, Y.; Wang, J. Roughening the White OLED Substrate's Surface Through Sandblasting to Improve the External Quantum Efficiency. Organic Electronics 2011, 12, 648–653.

Phosphorescent Exciplexes

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The steady state and time dependent photoluminescence spectra have been studied to determine whether the formation of a charge transfer state occurs between pairs of various organic molecules at both room temperature and the low temperature of 80K. Samples of these molecules were prepared on transparent quartz substrates in the form of thin films of the desired molecules which were prepared by dissolving in toluene, mixed in the desired ratios, pipetted onto the substrate and heated in a vacuum oven. The use of a fluorometer fluorolog, cryostat and ultra-fast 4 PICOS gated iCCD camera system with pulsed Nd:YAG laser at 355nm were used for the steady state measurements, the cooling of the samples and the time dependent measurements respectively with the aim of creating an organic exciplex system which displayed signs of phosphorescent emission. Various ratios of acceptor to donor volume were tested in ratios of 80 : 20, 70 : 30, 50 : 50 and the reverse. Evidence of charge transfer formation was found across several of the pairs of organic acceptor and donor molecules tested via the redshift and broadening of their emission peaks compared to their individual emission peaks. Only one sample, 0,10-Dimethyl-9,10-dihydroanthracen-9-on (DMA) mixed with 1- (tert-butyl)-10H-phenothiazine (PTZ-tBu) displayed firm evidence of strong phosphorescence emission. In addition, the samples showing evidence of a charge transfer state were compared to the same component molecules covalently bonded together to determine the difference in photophysical properties. It was concluded that charge transfer states display evidence of different photophysical properties, and hence different singlet and triplet energy levels.

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References

Gould, I. R., Boiani, J. A., Gaillard, E. B., Goodman, J. L., & Farid, S. (2003). Intersystem Crossing in Charge-Transfer Excited States. The Journal of Physical Chemistry A, 107(18), 3515–3524. https://doi.org/10.1021/jp022096k

Preliminary Photophysical Investigation of a Naturally Derived Luminophore: Green Extraction, Aggregation Dynamics, and Enhanced Room-Temperature Phosphorescence in Poly(acrylic acid) Matrix.

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The development of sustainable luminescent materials from renewable resources is an attractive strategy for designing eco-friendly photonic technologies. In this work, a natural luminophore was obtained through a simple cold-extraction protocol, avoiding high-energy processing and harsh chemicals, providing a green route for preparing photoluminescent materials in water. The photophysical properties of the extract were investigated in solution to understand the relation between molecular organization and excited-state behavior. A binary solvent system of water and tetrahydrofuran (THF) was employed to systematically modulate the polarity and microenvironment around the chromophore. Owing to the hydrophilic nature of the extract, gradual addition of THF induced changes in solvent quality, promoting molecular self-assembly and aggregation. These structural changes were monitored through steady-state photoluminescence spectroscopy, revealing that emission characteristics depend strongly on solvent composition and aggregation state. To explore confinement effects and suppress non-radiative deactivation, the luminophore was incorporated into poly(acrylic acid) (PAA) matrices. Remarkably, the rigid polymeric environment promoted intense room-temperature phosphorescence (RTP), indicating efficient stabilization of triplet excited states. This RTP behavior is attributed to molecular immobilization, restricted vibrational relaxation, and protection from oxygen quenching provided by the hydrogen-bond-rich PAA network. These results demonstrate that green extraction combined with polymer-assisted confinement is a promising strategy for sustainable RTP materials, opening opportunities for eco-friendly photonic devices.

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References
WANG, Tiantian et al. Recent advances in long-persistent luminescence materials based on host–guest architecture. Chinese Chemical Letters, v. 35, n. 1, p. 108385, 2024.

JI, Lukang et al. Protonation induced symmetry-breaking and fluorescence switching in C3-symmetric self-assemblies with application in optical information encryption. Journal of

Colloid and Interface Science, p. 138448, 2025.

LIU, Bifang et al. Isomeric design of carbazole and benzoindole derivatives for ultralong organic room-temperature phosphorescence. Dyes and Pigments, p. 113137, 2025.

Spatially resolved phonon lifetime evolution under pulsed laser perturbation in radiation-damaged crystalline systems

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Raman linewidth is directly related to phonon lifetime and structural disorder in crystalline materials [1]. Pulsed laser ablation, widely used in materials processing and compositional analysis, can locally perturb the lattice through transient heating and defect generation [2]. Yet, a quantitative description of the resulting structural gradients and their spectroscopic signatures remains incomplete. In this ongoing study, we examine the spatial evolution of Raman-active phonon linewidths as a function of distance from pulsed laser ablation craters in radiation-damaged crystalline systems. High-resolution micro-Raman mapping with micrometric steps is used to extract full-width-at-half-maximum (FWHM) variations up to ~80 μm from the ablation center. Preliminary results indicate linewidth broadening near the crater, consistent with increased disorder and reduced phonon lifetimes. However, transient heating may also promote partial structural recovery via thermally activated defect recombination, leading in some cases to linewidth narrowing. The radial dependence of FWHM is being analyzed within a transient Gaussian thermal framework, where the temperature profile follows diffusive heat transport from a Gaussian excitation source [3]. Assuming a correlation between defect density and peak transient temperature, an exponential radial decay model is being tested against alternative functions. Statistical comparison of fits and correction for instrumental broadening are currently underway. The expected outcome is a physically constrained description of laser-induced structural gradients, providing a quantitative basis for interpreting Raman linewidth variations in laser-processed crystalline materials and related photothermally perturbed systems.

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References

M. Dubajic et al., PRX Energy 4, 033020 (2025)

I. Rigó et al., Sci. Rep. 15, 14469 (2025)

Y.N. Makov, Acoustical Physics 47, 333 (2001)

Study of γ-butyrolactone (GBL) as solvent for recycling Perovskite Solar Cells (PSCs)

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The global energy transition has driven the development of clean and sustainable technologies, with solar energy standing out as a promising alternative due to its abundance. In this scenario, perovskite solar cells (PSCs) emerge as a technology with great potential due to their high power conversion efficiency (PCE) and relative low production cost, which may even overcome the limitations of conventional silicon cells [1]. However, the presence of lead (Pb) in their composition and the degradation of the devices over time represent major challenges, especially regarding disposal and the generation of toxic waste, which threatens the environmental forecasts of this technology.

In this context, several recycling methods have been developed and studied in order to reduce the volume of waste and create routes to reuse the materials, optimizing the cost-benefit of this technology [2,3]. However, many of these methods frequently use N,N-dimethylformamide (DMF) as a solvent [3], which is recognized for its high toxicity and negative impacts on health and the environment, which contradicts the principles of sustainability. In this work we developed an alternative route for recycling perovskite solar cells using γ-butyrolactone (GBL) as the main solvent. The methodology promotes the recovery of lead and transparent conductive substrates (TCOs), in order to make the process safer and more environmentally friendly. This approach aims to contribute to the creation of a more sustainable life cycle for PSCs, aligned with the objectives of a circular economy and reduction of environmental impacts. Preliminary XRD results indicate that reaction time is critical, determining whether pure PbI_2 powder is isolated or a mixture of solids forms due to iodide extraction from solution. Current work evaluates perovskite film quality from evaporated, recovered PbI_2.

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References
FONSECA, André F. V. et al. Perovskites beyond efficiency: stability challenges from space to Earth. Energy Advances, 2026.

XIAO, Xun et al. Aqueous-based recycling of perovskite photovoltaics. Nature, p. 1-6, 2025.

CHEN, Bo et al. Recycling lead and transparent conductors from perovskite solar modules. Nature communications, v. 12, n. 1, p. 5859, 2021.

Commercializing Conformal Soft Electronics for Healthcare and Aged Care

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The human body is soft and dynamic; electronics have always been hard and rigid. This fundamental incompatibility limits the utility of conventional devices for pervasive monitoring. This presentation focuses on our solution: stretchable and wearable electronics, a revolutionary class of devices that seamlessly integrate with biological systems. Our decade-long effort has successfully transformed conventional devices into soft, unbreakable products thin enough to function as electronic skin, enabling ultra-conformal patches that mimic body functionality.

I will detail the fundamental research required to solve the crucial materials science hurdle: enabling this conformal performance by integrating high-performing rigid oxide electronics (e.g., for sensing and data processing) onto soft, elastomeric polymeric substrates (e.g., rubber platforms).

The final section will demonstrate the successful translation and commercialization of this technology with industry partners. I will highlight real-world applications across diverse sectors, including wearables for continuous health monitoring, nearables (such as sensors integrated into bedding), skin-adhered sensors for tracking harmful substances like UV radiation and nicotine levels, and point-of-need diagnostics that bring lab-quality analysis to the patient.



Biomimetic Electronic Polymers for Tissue-Interfaced Continuous Biosensing

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Keywords: Bioelectronics, Biosensing, OECT, Immune compatible

In vivo recording of biochemical information, such as metabolites, proteins, cytokines, and transcription factors, offers the most direct and information-rich window into biological processes and physiological status, from inflammation and immune dynamics to neural activity. Yet achieving continuous biochemical sensing at tissue interfaces with meaningful spatiotemporal resolution remains a major unsolved challenge. Current biosensing technologies face a wide spectrum of limitations, including mechanical invasiveness, poor tissue attachment, biofouling, chronic immune responses, and insufficient sensitivity for low-abundance biomarkers such as cytokines. My group has developed a series of biomimetic design concepts for semiconducting and conducting polymers, to realize a range of properties, including stretchability, tissue adhesion, surface adaptability, and immune compatibility. In addition, our recent report of hydrogel semiconductors as a new materials platform is realizing a new mode of 3D volumetric biochemical sensing that enables high sensitivity at low analyte concentrations. In this talk, I will introduce the design principles behind these bioelectronic materials and highlight our recent progress in achieving tissue-interfaced, continuous, and multiplexed biosensing with significantly extended in vivo stability. Moving forward, these biomimetic design principles for electronic polymers may lay the foundation for a new generation of adaptive, intelligent bioelectronic interfaces that continuously map the biochemical state of living systems.

Biorecognition across lengthscales with electrolyte gated organic transistors

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Keywords: biosensors, biorecognition, biomarkers

Biorecognition is the ability of biological molecules to selectively identify and bind specific targets, such as enzymes recognizing substrates or antibodies binding antigens. It underpins essential processes in life and is central to biotechnology, enabling applications like biosensors and related diagnostics advances, and targeted therapies through highly specific molecular interactions. Electrolyte Gated Organic Transistors (EGOTs) are now a well-established key player in the field of biosensing [1]. In recent years, they were demonstrated as ultra sensitive solutions for detection and quantification of a large portfolio of analytes, highlighting the platform character of this technology. A remarkable feature exhibited by the demonstrated EGOT based biosensors is their ability to transduce binding of targets that span a very large lengthscale range, from small molecules such as neurotransmitters and cholesterol to proteins, up to viruses and even exosomes. I will present the latest achievements of our group in the applications of EGOT for personalized medicine in complex samples, with a focus on the development of immunosensors for antidrug antibodies, involved in the response to immunotherapies, for phosphorylated Tau protein, an emerging biomarker for Alzheimer disease, detected in cerebrospinal fluids, and for the quantification of extracellular vesicles from breast cancer patients. Besides describing the analytical performances of the devices, I will focus on the models developed to correlate binding event to the device response through multiparametric analysis of the experimental transfer characteristics [2] and to elucidate binding equilibria at the gate/electrolyte interface [3].

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References:

[1] F. Torricelli, D.Z. Adrahtas, et al., *Nature Reviews Methodes Primers* **66**, 1, (2021)
[2] R. Zanotti, M. Berto, et al., *Advanced Materials* **36**, 2410940 (2024)
[3] M. Sensi, RF de Oliveira et al., *Advanced Materials* **35**, 2211352 (2023)

Conducting polymer devices for hosting and monitoring in vitro models of the gut

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Keywords: organic bioelectronics, PEDOT:PSS, conducting polymer, organ-on-chip

Physiologically relevant in vitro human models are urgently required to bridge the gap between over-simplified 2D in vitro models and ill-suited animal models, for drug discovery and disease modelling. 3D in vitro models are becoming more widespread but usually ill-suited to conventional monitoring techniques (largely microscopy) that generate continuous data. Bringing together principles of materials science, tissue engineering, 3D cell biology and bioelectronics, we are building advanced models of tissues. Our models are based on the use of electroactive scaffolds which can host tissues, but also monitor their formation in real time, and also their status when challenged or stimulated. Our strategy is to build a stromal layer with the scaffold and layer epithelial or endothelial models on top, preserving tissue stratification. We have adapted these scaffolds to the well-known Transwell format, to allowed continued access to both apical and basal aspects. As well as traditional readouts such as immunofluorescence, or biochemical analyses of media, continuous electrical monitoring readouts from our electroactive scaffolds gives us real-time data on the tissue health. In this presentation I will described our ongoing work focused on understanding the scaffold composition, morphology and materials characteristics both in terms of cell growth and proliferation, but also the effect on the electrical readout, via both electrical impedance spectroscopy (2 electrode configuration) and using an electrochemical transistor configuration (3 electrode configuration). I will also present our work on using conformal conducting polymer devices to monitor advanced models of the gut in vitro.



Figure 1: ICSM 2026 image

Light harvesting with organic molecular materials: insights from time-resolved spectroscopic studies

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Abstract

Efficient solar energy harvesting is fundamental for advancing future technologies, spanning from renewable energy devices to cutting-edge optoelectronic modules like OLEDs and solar-pumped lasers. Inspired by the high quantum efficiency of natural photosynthesis, researchers have developed various artificial systems for a range of applications. Optimizing these materials demands a deep understanding of their structure-function relationships and a multidisciplinary approach, with time-resolved spectroscopy playing a crucial role in unraveling complex photoinduced dynamics.

In this presentation, I will discuss our recent studies on different classes of molecular materials based on small organic molecule building blocks, focusing on their light-induced dynamics. Examples include organic materials used as Luminescent Solar Concentrators (LSCs), which have recently emerged as key tools for visible light wireless communications, and self-assembled conjugated aggregates designed as light-harvesting media for OLEDs and polaritonic devices.

Organic Retinomorphic Imager and Electrochemical Transistor for Environmental Monitoring

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Fast, low-power motion capture is essential for applications in machine vision and environmental monitoring. This work presents a reconfigurable retinomorphic device that can be electrically switched between two complementary operating modes: a motion mode that delivers streamlined spiking signals for efficient motion tracking, and a static mode that integrates charge to capture high-fidelity images. Mode switching is achieved at the device level by tuning the variable resistance within a photocapacitor–transistor architecture. This work also establishes measurement guidelines for time-derivative sensors to evaluate rate-dependent detection limits. To demonstrate scalability and integration capability, 8 × 8 pixel arrays are fabricated, enabling spatiotemporal imaging in dual modes. This device-level approach reduces circuit overhead traditionally required for multimodal operation and offers a compact configuration for reducing energy consumption and facilitating high-density integration in next-generation vision systems.

Performance Enhancement in Mixed Ionic-Electronic Conductors by Molecular Design, Blend and Architecture Engineering

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Keywords: OMIEC, OECT, organic, neuromorphic, blend, transport

In this presentation we report the development of novel ionic-electronic molecular and polymeric ionic-electronic conductors and their implementation in various devices. First, we summarize recent results where a new vertical electrochemical transistor architecture is reported enabling excellent electronic transport for several polymer semiconductors. Next, from the material development we report the synthesis of new n-type molecular materials designed to have ionic channels for efficient ion intercalation. Furthermore, we report a family of NDI and DPP polymers where electrochemical transistor performance is manipulated by the backbone structure, functionalization and device architecture. In addition, we discuss recent implementation of a new n-type polymers for the realization of high-performance and balanced complementary electrochemical OECTs and inverters, which are then used to fabricate neuromorphic circuits capable of sensing, transducing and recording information. Finally, we report our recent stategy based on blending hydrophilic additives to hydrophobic semiconductors.

References:

[1] Gao, Lin. ; Cho, Y.; Wang, R.; Yao, Y.; Zhang, D.; Wang, Y.; Cheng, Y.; Wang, Y.; Ma, Q.; Duplessis, I.; Chung, S.; Wilson, E.; Cho, K.; Wang, B.; Li, B.; Rivnay, J.; Wang, H.; Yu, J.; Facchetti, A. Broadly applicable hydrophilic additive enhances electrochemical transistor function *Proceedings of the National Academy of Sciences* **2026**, *123* (10) e2523877123

[2] Yao, Y.; Pankow, R. M.; Huang, W.; Wu, C.; Gao, L.; Cho, Y.; Chen, J.; Zhang, D.; Sharma, S.; Liu, X.; Wang, Y.; Peng, B.; Chung, S.; Cho, K.; Fabiano, S.; Ye, Z.; Ping, J.; Marks, T. J.; Facchetti, A. An organic electrochemical neuron for a neuromorphic perception system. *Proceedings of the National Academy of Sciences* **2025**, *122* (2), e2414879122. DOI: doi:10.1073/pnas.2414879122.

[3] Cho, Y.; Gao, L.; Yao, Y.; Kim, J.; Zhang, D.; Forti, G.; Duplessis, I.; Wang, Y.; Pankow, R. M.; Ji, X.; et al. Small-Molecule Mixed Ionic-Electronic Conductors for Efficient N-Type Electrochemical Transistors: Structure-Function Correlations. *Angewandte Chemie International Edition* **2025**, *64* (2), e202414180. DOI: https://doi.org/10.1002/anie.202414180.

[4] Kim, J.; Pankow, R.; Cho, Y.; Duplessis, I.; Qin, F.; Meli, D.; Daso, R.; Zheng, D.; Huang, H.; Rivnay, J.; Marks, T. J.; Facchetti, A. Monolithically integrated ultra-high-density vertical organic electrochemical transistor arrays and complementary circuits *Nat. Electron.* **2024**, DOI: 10.1038/s41928-024-01127-x

Plasmonic Nanomaterials as Dual-Action Agents for Light-Triggered Cancer Therapy

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Our group has been developing nanoengineered materials for photodynamic (PDT) and photothermal (PTT) therapies, with emphasis on plasmonic systems that integrate light-to-heat conversion with photoinduced oxidative damage. In this presentation, we will briefly introduce this research line and then highlight a representative study using shell-isolated gold nanorods functionalized with toluidine blue O (AuSHINRs@TBO) as a dual-function platform for colorectal cancer treatment. The phototherapeutic effect was evaluated in human colorectal adenocarcinoma cells (Caco-2). Under irradiation, AuSHINRs induced heat-mediated cytotoxicity due to localized surface plasmon resonance (LSPR). TBO functionalization significantly increased the phototoxic response, indicating PTT/PDT synergy. MTT assays showed a decrease in cell viability from 85.5% (AuSHINRs) to 39.0% (AuSHINRs@TBO) after irradiation, consistent with an additional oxidative damage pathway. To investigate the interfacial mechanism, Langmuir monolayers prepared from Caco-2 lipid extracts were used as a biomimetic membrane model. Surface pressure-area isotherms and PM-IRRAS indicated electrostatic interaction of the nanoconjugates with anionic lipid headgroups, leading to monolayer expansion. After irradiation, AuSHINRs@TBO-containing monolayers showed an ~1% increase in molecular area, suggesting ROS-mediated lipid oxidation and membrane perturbation. Confocal fluorescence microscopy supported membrane disruption as a major event in photoinduced cell death. Together, these results show that AuSHINRs@TBO is an effective synergistic phototherapeutic platform and reinforce the importance of membrane-targeted mechanisms in colorectal cancer phototherapy.

Polymer nanoparticles optically control the cell fate

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The capability to control and modulate the activity of biological systems is considered a major target in biomedical technology research, because it can lead to a deeper understanding of specific functions and to innovative strategies to manage dysfunctions. Modulation by means of light reduces invasiveness of treatment and allows to achieve reversibility and high spatial and temporal resolution. Since however living cells are transparent to light, it is necessary to make recourse either to optogenetic tools, based on viral transfection of light-sensitive proteins, or to light-sensitive smart materials.

Conjugated polymers are optimal candidates for the latter approach, due to their peculiar optoelectronic properties combined with the chemical and mechanical advantages of organic materials. Some recent works have demonstrated their excellent reliability in the modulation of excitable cells, tissues and even animal behaviour. Conversely, this approach has been very rarely adopted in the case of non-excitable cells. In particular, the possibility to optically modulate cell fate and metabolic processes has never been considered. This work represents a first attempt towards this ambitious goal.

We report on the fabrication, engineering and chemical/physical characterization of several kinds of biocompatible, organic semiconducting nanoparticles. The functional interaction between polymer beads, optical excitation and living systems has been studied in a number of different biological models, including cardiac, endothelial and epithelial cells. We discuss in detail more relevant results in the understanding of the phototransduction mechanisms, able to trigger effective modulation of calcium ion flux and to modulate the intracellular redox balance. Our targeted applications are in the fields of regenerative medicine, skin repair, cardiac tissue engineering. Here, we will show in vitro and in vivo data on the use of polymer nanoparticles for different therapeutic purposes, including wound healing, skin regeneration, angiogenesis and cardiac stenosis.

Polymeric Mixed Conductors for Bioelectronic Sensors

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Organic mixed ionic and electronic charge conductors offer a unique toolbox for establishing electrical communication with biological systems. In this talk, I will introduce this rising class of materials for bioelectronic interfacing and explain how their multifunctionality can be harnessed to develop next-generation conformable bioelectronic sensors operating at aqueous electrolyte and tissue interfaces. I will highlight one application where organic electrochemical transistors that rely on these soft conductors are used to detect biochemical molecules from sweat while recording and analyzing electrophysiological signals. Drawing from our experience with patient samples, I will address potential shortcomings of proof-of-concept biosensor platforms and explore strategies for overcoming these challenges.

Resorbable organic semiconductor devices for post-surgical monitoring

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Organic semiconductors enable a variety of novel applications for flexible, lightweight, and environmentally friendly electronics. One unique advantage of these carbon-based materials is their compatibility with body tissue, thus opening perspetives for new medical applications on or even in the human body. Furthermore, the materials set available in this technology allows biodegradability and thus sustainable electronics without the serious environmental issue of conventional electronics. In my talk, I will discuss an example how organic electronic devices can be used in post-surgical monitoring of anastomosis insufficiency (leakage of reconnected intestine sections), avoiding life-threatening complications. The devices, which are inserted as a ring into the reconnections of the intestine, monitor when an insufficiency occurs [1]. They are realized on polydioxanone substrates, a material which has been used for resorbable suture threads for decades. The anastomosis insuffiency is detected by tracking the impedance of the detectors envirnment. In animal tests, a clear signal related to the insuffiency is observed. I will also describe remaining challenges towards usage in humans and other opportunities for this kind of technology.

I thank my coworkers in Dresden and Rostock, in particular Finn Jaekel and Dennis Wahl, for the very enjoyable collaboration.

[1] Real-Time In Vivo Monitoring of Anastomotic Intestinal Ischemia Using Implantable Resorbable Organic Sensors, D. Wahl, F. Jaekel, et al., Advanced Science 2025, e14507

The Road to “Green” in Organic Bioelectronics

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Through its appealing avenues of processing the component devices at room temperature and from low-cost precursor materials, organic electronics has a tremendous potential for the development of products able to achieve the goals of production sustainability as well as environmental and human friendliness for electronics.

In an effort to stave off the e-waste growth, the presenter and his research group went further down the path opened by organic electronics research and investigated a large number of biomaterials as substrates, dielectrics, semiconductors and smoothening layers for the fabrication of organic field effect transistors, integrated circuits and organic solar cells. The presentation will focus on the highlights of our recent research, especially with respect to materials investigated, devices fabricated and the immense potential for follow up research: (1) flexible natural and biodegradable substrates; (2) natural dielectrics; (3) bio-origin, H-bonded semiconductors in the families of indigos, anthraquinones and acridones; (4) bio-degradation protocols for organic semiconductors.

These highlights will be placed in the context of the mountain that one has to climb in order to reach the coveted “green” connotation for electronics, sensors and integrated circuits: (1) biocompatibility issue; (2) biodegradability issue; (3) compostability issue; (4) cost of production / energy expanded in production issue; (5) materials choice issue (carbon foot print); (6) toxicity and the environmental impact of the synthetic avenue for component materials.

The potential of follow-up research in the green electronics field is immense, with large area electronics fabrication, biomedical implants, bio-sensing and smart labeling, representing only the tip of the iceberg of many more immediate possibilities of high interest for our group. Natural and nature-inspired materials have the unrivalled capability to create “safe first” electronic markets for human and environment.

Wireless Piezoelectric Stimulation of Cells via Ultrasound-Responsive Polymeric Nanomaterials

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Piezoelectric stimulation is emerging as a powerful strategy to modulate cellular behavior by converting mechanical energy into localized electrical cues. This approach enables wireless, noninvasive, and spatially controlled bioelectronic stimulation, overcoming key limitations of conventional electrode-based systems. Here, we present recent advances from our group on the development and biological application of piezoelectric nanomaterials for ultrasound-driven cell stimulation.

We report the design and characterization of organic piezoelectric nanoparticles able to transduce low-intensity ultrasound into bioactive electrical signals. Using polymeric and polysaccharide-based nanotransducers, including biodegradable chitosan nanoparticles and piezoelectric fluoropolymer nanoparticles, we demonstrate effective mechano-electrical coupling at the nanoscale. Upon ultrasound activation, these systems generate localized electrical and electrochemical effects that modulate intracellular signaling without the need for exogenous drugs or genetic manipulation.

Biological studies show that piezoelectric stimulation induces sustained calcium dysregulation and reactive oxygen species generation, leading to marked functional outcomes. In patient-derived glioblastoma models, chronic ultrasound-driven piezostimulation produces strong antiproliferative and proapoptotic effects, validated in both 2D cultures and ex ovo tumor models [1]. In parallel, in human neural stem cells, the same stimulation paradigm promotes exit from the cell cycle, neuronal differentiation, and enhanced neurite outgrowth through calcium-dependent, growth-factor-independent mechanisms [2].

Overall, these results identify piezoelectric nanomaterials as a versatile and clinically relevant platform for remote cell stimulation, with potential applications spanning oncology and neuroregeneration.

[1] Marino A., Curiale T., Lefevre M.C., Carmignani A., Ceccarelli M.C., Battaglini M., Ziaja K., Marras S., Torre B., Fiaschi P., Ciofani G. Ultrasound-activated biodegradable piezoelectric chitosan nanoparticles for glioblastoma treatment. Small Science, 10.1002/smsc.202500457

[2] Bargero A., Battaglini M., Curiale T., Carmignani A., Montorsi M., Labardi M., Pucci C., Marino A., Ciofani G. Ultrasound-responsive polymeric piezoelectric nanoparticles for remote activation and neuronal differentiation of human neural stem cells. Small Science, 5(2): 2400354 (2025)

A Nanotube-Confined Tellurium Neuromorphic Visual System for Image Processing and Reservoir Computing

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Biological vision systems integrate perception, memory, and processing functions into compact and energy efficient architectures, inspiring the development of neuromorphic optoelectronic devices. However, most existing artificial vision systems rely on external gate modulation, complex circuitry, or multiple heterogeneous materials, limiting their energy efficiency, stability, and large scale integration. Here, a neuromorphic two terminal optoelectronic resistive random access memory (ORRAM) visual system based on tellurium/carbon nanotube (Te@CNT) low dimensional materials is presented, which integrates optical sensing, information storage, and image preprocessing. Benefiting from strong interfacial coupling and band bending at the Te@CNT heterointerface, the device operates at a bias as low as 0.1 V and exhibits photoresponses to ultraviolet ligh and visible light. Under optical modulation, the device exhibits tunable synaptic dynamics, including nonlinear optical response and short term and long term plasticity, and is able to classify 16 binary inputs to achieve physical reservoir calculations. Furthermore, the Te@CNT ORRAM array integrating artificial neural networks exhibits image preprocessing capabilities, such as contrast enhancement, background denoising, and image erasure. For letter image recognition, an accuracy of over 99% is achieved in just 10 training epochs. This work presents a compact and low power neuromorphic visual platform, highlighting the great potential of carbon nanotube confined low dimensional materials for next generation intelligent optoelectronic systems.

Acknowledgements
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References
[1] G. Zhou, J. Li, Q. Song, L. Wang, Z. Ren, B. Sun, X. Hu, W. Wang, G. Xu, X. Chen, L. Cheng, F. Zhou, S. Duan, Full hardware implementation of neuromorphic visual system based on multimodal optoelectronic resistive memory arrays for versatile image processing, Nature Communications, 14 (2023) 8489.

[2] Y. Kim, A. Chortos, W. Xu, Y. Liu, J.Y. Oh, D. Son, J. Kang, A.M. Foudeh, C. Zhu, Y. Lee, S. Niu, J. Liu, R. Pfattner, Z. Bao, T.-W. Lee, A bioinspired flexible organic artificial afferent nerve, Science, 360 (2018) 998-1003.

[9] Z. He, H. Duan, J. Zeng, J. Zhou, X. Zhong, Z. Wu, S. Ni, Z. Jiang, G. Xie, J.-Y. Lee, Y. Lu, Y. Zeng, B. Zhang, W.B. Ying, Z. Yang, Z. Zhang, G. Liu, Perovskite retinomorphic image

sensor for embodied intelligent vision, Science Advances, 11 (2025) eads2834.

A Versatile, Biomimetic, 3D Electrochemical Device for Monitoring Cell Growth and Epithelial Barrier Integrity

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Three-dimensional (3D) cell culture and in-vitro bioelectronic systems have advanced significantly in recent years, offering new capabilities for monitoring and predicting biological activity in a variety of applications. While bioelectronic devices such as impedance sensors and electrochemical transistors have traditionally been based on two-dimensional (2D) organic semiconductor films, tissue engineering has developed 3D culture platforms—such as porous scaffolds, hydrogels, and fibre meshes—that better replicate native tissue architecture and physiology. In this work, we present a novel bioelectronic device that integrates these two domains. The device is built around a 3D microporous scaffold based on the conducting polymer PEDOT:PSS, serving both as a biologically relevant substrate and as an active electronic interface. The scaffold functions as a transmembrane structure that hosts multiple cell types, enabling the formation of stratified tissue models, while simultaneously transducing biological (ionic) signals into readable electrical outputs. We demonstrate the design, fabrication, and electrical characterization of this transmembrane bioelectronic platform, which combines dual sensing modalities: electrochemical impedance spectroscopy (EIS) for monitoring epithelial barrier formation and integrity, and organic electrochemical transistor (OECT) operation for real-time tracking of cell growth and extracellular matrix (ECM) deposition in 3D. Using fibroblast cultures as a model, we monitored tissue development over a 10-day period. Changes in drain current provided a quantitative readout of cell proliferation and ECM accumulation. We evaluated the influence of initial seeding densities (125k, 250k, and 500k cells), observing distinct patterns of cell migration, proliferation, and matrix remodeling, which were corroborated with biological assays including immunofluorescence imaging and DNA quantification.

References

C. Pitsalidis, D. van Niekerk, C.M. Moysidou, A.J. Boys, A. Withers, R. Vallet, R.M. Owens, Sci. Adv. 8 (2022) eabo4761.

Bioinspired redox membranes for stable, high-charge-injection organic electrodes

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The development of organic bioelectronic interfaces calls for materials that combine redox activity, mixed ionic–electronic transport and biocompatibility. Catechol chemistry offers a powerful bioinspired platform for designing such systems, enabling reversible redox processes and strong interfacial interactions. However, translating catechol-based materials into stable and efficient electrode architectures remains a major challenge.
Here we introduce a fully organic redox-active membrane obtained by interfacial polymerization between catechol and aromatic amine building blocks, forming a crosslinked network with intrinsic electrochemical functionality. The interfacial approach enables the formation of free-standing, structurally asymmetric membranes and provides a versatile route to integrate catechol redox units within an extended organic framework.
A key feature of this system is its electrochemical activation: upon potential cycling, the initially poorly conductive film evolves into a stable, delocalized redox network capable of supporting efficient charge transport. This transformation unlocks the full electrochemical functionality of the catechol-based polymer, enabling its use as an electrode material.
The resulting organic bioelectrodes exhibit low impedance, high charge storage and efficient charge injection under physiologically relevant conditions. Notably, their performance approaches that of benchmark materials such as gold and PEDOT, while offering the advantages of a fully organic, soft and bioinspired interface.
These results highlight catechol-based redox polymers as a promising platform for next-generation bioelectronic devices, bridging organic materials chemistry and neural interfacing. Building on our group's established catechol-based membrane platform [1-3], we are now modulating its redox properties to expand its applicability in bioelectronics.

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References
[1] Bolaños-Cardet, Pepió-Tárrega et al., Angew. Chem. 138(3), e13698 (2026).

[2] Bolaños-Cardet J., Pugliese S., Bruna J., Ruiz-Molina D., Yuste V.J., Suárez-García S.,

Adv. Sci. (2026).

[3] Contreras-Pereda N., Suárez-García S., Pfattner R., Ruiz-Molina D., Mater. Today Chem. 35, 101855 (2024).

Dissipative Charge Transport and Electrochemical Strain Waves in Organic Mixed Ionic-Electronic Conductors for Bioelectronics

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Understanding charge transport in organic mixed ionic-electronic conductors (OMIECs) is crucial to improve the performances of bioelectronic and neuromorphic devices. Recent studies reveal that the amplification of electrical signals in organic electrochemical transistors is determined by the volumetric capacitance cv and electronic mobility μ of OMIEC channels [1], but how material parameters impact on the signal propagation speed and energy dissipation remains unclear. To address this issue, we combine electrical measurements of the phase velocity in microstructured OMIEC channels with local measurements of electrochemical strain wave propagation with modulated electrochemical atomic force microscopy[2]. We interpret experimental data with a simplified transmission line model to determine the dispersion relation for OMIEC channels. We demonstrate that at relevant frequencies the phase velocity is dominated by the ratio of μ/cv, constituting an additional figure of merit to benchmark material formulations [3]. These results highlight intrinsic limitations of OMIEC-based circuits and compare their efficiency with neuronal signal transmission.

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References
F. Bonafè, F. Decataldo, I. Zironi, I, D. Remondini, T. Cramer, B. Fraboni, " AC amplification gain in organic electrochemical transistors for impedance-based single cell sensors.", Nat Commun 13, 5423 (2022)

F. Bonafè, J. Ji, S. Fabiano, B. Fraboni, and T. Cramer, “ Investigation of Transport in OECTs with Electrochemical Strain Wave Microscopy.”, Small 21, no. 52 (2025)

F. Bonafè, M. Bazzani, B. Fraboni, and T. Cramer, "Dissipative charge transport in organic mixed ionic-electronic conductor channels.", Nat Commun 16, 2499 (2025)

Excited State Opto-Ionic Reservoir Computing in Hybrid Perovskite Electrochemically-Gated Luminescent Cells

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We present a physical reservoir computing concept that harnesses the coupled electronic–ionic dynamics of lead-halide perovskites. Photogenerated defects link photoexcited charge carriers to ionic motion, while the heterogeneous microstructure and excited-state processes generate a high-dimensional, adaptive internal state space. This enables fully all-optical reservoir computing with spatially resolved photoluminescence used for readout. The system processes temporal pulse patterns and successfully tackles nonlinear time-dependent benchmarks such as NARMA2, demonstrating robust performance well suited to neuromorphic tasks. Using physics-informed machine learning, we further reveal how defect-mediated opto-ionic interactions shape the underlying spatio-temporal dynamics. Beyond benchmarking, the approach suggests promising applications in machine vision, edge computing, and other resource-constrained intelligent systems, highlighting excited-state physics in photoactive materials as a compelling pathway toward nanoscale neuromorphic technologies.

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References
P.Kollenz, C.Herrle, L.Göhringer, et al. “Excited State Opto-Ionic Reservoir Computing in Hybrid Perovskite Electrochemically-Gated Luminescent Cells.” Advanced Materials38, no. 14 (2026): e12575. https://doi.org/10.1002/adma.202512575

Interfacial Mechanics of Acetogenins in Tumor Membrane Models: the Impact of Chain Unsaturation

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Acetogenins are natural products with reported bioactivity against microbial pathogens and tumor cells. Recently, acetylenic acetogenins isolated from Porcelia macrocarpa have drawn attention due to clear structure–activity relationships [1]. In particular, cytotoxicity correlates with alkyl chain unsaturation: highly unsaturated derivatives are biologically active, whereas saturated analogues show little or no activity. Understanding how these structural differences affect membrane interactions is key to elucidating their mechanism of action.

Here, we investigate the interfacial behavior of three acetogenins (ACGs 1–3) using tumor membrane models based on Langmuir monolayers. Films of dipalmitoylphosphatidylserine (DPPS) were formed at the air–water interface to mimic the outer leaflet of tumor cell membranes. ACGs (10 mol%), including an equimolar mixture of ACGs 1 and 2, were co-spread with DPPS. The films were characterized by surface pressure–area isotherms, compressional modulus, hysteresis cycles, kinetic stability, dilatational rheology, Brewster angle microscopy (BAM), and PM-IRRAS.

Unsaturated acetogenins significantly disrupt and destabilize the monolayers, unlike the saturated analogue. ACG 1 shows the strongest effect, promoting molecular reorganization at biologically relevant surface pressures and reducing film elasticity. Spectroscopic and morphological data indicate interactions with lipid alkyl chains, increasing disorder and fluidity.

These results provide mechanistic insight into acetogenin–membrane interactions, highlighting the role of chain unsaturation in modulating interfacial behavior and bioactivity, with implications for the design of bioactive amphiphilic materials.

Acknowledgements
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References
I. A. Brito et al. Antileishmanial effects of acetylene acetogenins from seeds of porcelia macrocarpa (Warm.) R.E. Fries (annonaceae) and semisynthetic derivatives. Molecules, 2022, v. 27, n. 3, p. 893.

Langmuir–Blodgett Thin-Film Immobilization of Urease Hybrid Nanoflowers for Capacitive Urea Biosensing

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Biosensors have been widely investigated for the detection of diverse analytes. Due to their high selectivity and catalytic efficiency, enzyme-based biosensors are attractive as cost-effective platforms for monitoring compounds relevant to human health and industry, such as urea. In this context, enzyme hybrid nanoflowers (EHN) have emerged as promising materials because they combine enhanced catalytic performance with high surface area compared to free enzymes. Although EHN synthesis and applications are well documented, their immobilization onto organized solid supports remains scarcely explored. Here, urease–$Cu_3(PO_4)_2$ hybrid nanoflowers were immobilized in organized thin films using the Langmuir–Blodgett (LB) technique. Monolayers composed of dimyristoyl phosphatidic acid (DMPA), poly(9,9-dioctylfluorene-co-phenylene) (PFPh), and EHNs were transferred onto quartz and silicon substrates to fabricate multilayered architectures. Quartz crystal microbalance measurements confirmed EHN incorporation and stability. Seven-layer LB films exhibited catalytic activity following Michaelis–Menten kinetics, with KM = 7.96 mM and Vmax = 0.0146 mmol min^{-1}. Scanning electron microscopy indicated EHN incorporation within internal layers, suggesting effective entrapment and structural preservation. The LB films were integrated into electrolyte–insulator–semiconductor (EIS) capacitive structures to evaluate biosensing performance. Capacitance measurements revealed a clear urea response due to enzymatic hydrolysis and subsequent interaction of OH^- ions with the Ta_2O_5 sensing layer. While DMPA and DMPA/PFPh films showed negligible sensitivity, EHN-containing films exhibited a linear response with a sensitivity of 9.00 ± 0.91 mV $decade^{-1}$ and a detection limit of 0.305 µmol L^{-1}. These results demonstrate a robust strategy for immobilizing EHNs in organized thin films and highlight their potential for next-generation biosensing platforms.

Acknowledgements
INEO, Capes and FAPESP (grant number 2025/27044-5; 2024/14903-7)

References

C. G. de Jesus, R. da Rocha Rodrigues, L. Caseli, and L. O. Péres, “Conducting polymers modulating the catalytic activity of urease in thin composite films,” Colloids Surfaces A Physicochem. Eng. Asp., vol. 654, pp. 130136, 2022, doi: 10.1016/j.colsurfa.2022.130136.

J. Ge, J. Lei, and R. N. Zare, “Protein-inorganic hybrid nanoflowers,” Nat. Nanotechnol., vol.

7, no. 7, pp. 428–432, 2012, doi: 10.1038/nnano.2012.80.

Near-Infrared Phototherapeutic Nanoplatforms Based on Gold Shell-Isolated Nanoparticles for Targeting Cancer Cells

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Leukemia is characterized by the uncontrolled proliferation of abnormal white blood cells and demands therapeutic strategies capable of selectively eliminating malignant cells while minimizing systemic toxicity. Photothermal therapy (PTT) and photodynamic therapy (PDT) are minimally invasive, light-triggered approaches that induce localized cytotoxicity through heat generation and reactive oxygen species (ROS) production, respectively. When combined, these modalities can act synergistically through complementary mechanisms, enhancing therapeutic efficacy. Herein, gold shell-isolated nanostars (AuNS@SiO_2) were synthesized and conjugated with indocyanine green (ICG), followed by deposition of a second silica shell to obtain AuNS@SiO_2-ICG-SiO_2 nanostructures. This architecture enables near-infrared (NIR) activation and promotes spectral overlap between the localized surface plasmon resonance of the gold nanostars and the ICG absorption band, allowing simultaneous photothermal and photodynamic excitation under a single wavelength (at 810 nm). Physicochemical characterization confirmed successful ICG incorporation and silica encapsulation, evidenced by a plasmon red shift (830 to 835 nm), increased hydrodynamic diameter (109.9 to 135.7 nm), and higher ζ-potential (40.76 to 44.19 mV). Under 810 nm irradiation (28.05 mW cm^{-2}), the hybrid nanoplatform exhibited enhanced photothermal heating and singlet oxygen ($^1O_2$) generation compared to AuNS@SiO_2 and free ICG, demonstrating synergistic photothermal and photodynamic performance. In acute myeloid leukemia (HL-60) cells, flow cytometry revealed time-dependent nanoparticle uptake. Following NIR photoactivation, AuNS@SiO_2-ICG-SiO_2 induced a 62% reduction in cell viability (1:4 volumetric ratio), whereas AuNS@SiO_2 alone showed negligible cytotoxicity. These results highlight the potential of this NIR-responsive nanoplatform for synergistic phototherapy of acute myeloid leukemia.

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References

H. Döhner, et al. Blood 2017, v. 129, n. 4, p. 424–447.

M. Overchuk, et al. ACS Nano 2023, v. 17, n. 9, p. 7979–8003.

Recalibration-Free Multi-Day Wearable Electrophysiology Using Carbon Nanotube Dry Electrodes

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Wearable electrophysiology systems rely critically on stable, low-impedance interfaces between electronic sensors and the skin. Conventional wet electrodes provide high signal quality but degrade rapidly due to gel dehydration and skin irritation, while existing dry electrodes often suffer from high impedance, motion artifacts, and unstable signal characteristics that require frequent recalibration in machine-learning–driven applications. We present ultrathin dry bioelectrodes based on carbon nanotube (CNT) thin films that enable stable, high-fidelity electrophysiological recordings over multi-day timescales. The CNT films are synthesized through a scalable roll-to-roll floating catalyst chemical vapor deposition process capable of producing more than 10 m^2 of CNT film per hour, enabling large-scale manufacturing of breathable, conformal electrodes. The resulting nanostructured CNT networks exhibit sheet resistances below 250 Ω/sq, maintain electrical stability under 30% strain for over 2000 mechanical cycles, and possess high breathability with a water vapor transmission rate of 4.9 mg cm^{-2} h^{-1}, comparable to open-air conditions. By optimizing the balance between conformability, network density, and sheet resistance, we achieve an optimal electrode configuration at ~65% optical transmittance, resulting in skin–electrode contact impedance three times lower than conventional wet Ag/AgCl electrodes. The electrodes enable high-quality recordings across multiple electrophysiological modalities including EMG, EEG, and ECG. In EMG measurements, CNT electrodes achieve signal-to-noise ratios up to 80.6 ± 2.6 dB, significantly exceeding wet electrode performance. We implemented a multi-day myoelectric interface in which CNT electrodes were worn continuously for 48 hours while controlling a two-dimensional cursor using a Kalman filter decoder. The system maintained stable decoding performance without model recalibration, representing the first demonstration of a dry electrode

References

Moin, A., Zhou, A., Rahimi, A. et al. A wearable biosensing system with in-sensor adaptive machine learning for hand gesture recognition. Nat Electron 4, 54–63 (2021). https://doi.org/10.1038/s41928-020-00510-8

Reservoir Computing using Organic Mixed Ionic Electronic Conductors

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Reservoir computing (RC) is a promising paradigm for machine learning that utilizes dynamic systems, termed as reservoirs, to process and analyze complex temporal data. Organic mixed ionic electronic conductors (OMIECs) have emerged as a novel class of materials with intriguing properties, such as their ability to exhibit both electronic and ionic conductivity, as well as their biocompatibility, flexibility, and low power consumption. These features make OMIECs particularly suitable for the development of unconventional computing architectures in the field of bioelectronics. We present recent findings interlinking electronic conductivity, system nonlinearity and reservoir size with the neuromorphic functionality and RC performance of self-organized and structured OMIEC reservoirs. This study includes novel insights into the differences and similarities of p-type, n-type and ambipolar semiconductors in terms of operation speed and energy consumption. The recent progress in reservoir computing using organic mixed ionic electronic provides valuable knowledge for the targeted development OMIEC reservoirs. Given these findings, we are confident to further advance OMIEC based reservoirs to specific application scenarios, paving the way to future commercialization.

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References
Matteo Cucchi et al. ,Reservoir computing with biocompatible organic electrochemical networks for brain-inspired biosignal classification.Sci. Adv.7,eabh0693(2021).DOI:10.1126/sciadv.abh0693

Single-Transistor Organic Electrochemical Neurons for Dense, Flexible, and Bio-Realistic Neuromorphic Systems

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Neuromorphic bioelectronics seeks to emulate neuronal dynamics within ionic environments to enable seamless integration with biological systems. However, conventional silicon-based platforms are inherently incompatible with electrolytes and lack the biocompatibility required for stable biointerfaces. Organic mixed ionic–electronic conductors (OMIECs) provide a compelling alternative, yet most reported organic artificial neurons rely on multi-component circuit architectures, limiting integration density and scalability. Here we present a single-transistor organic electrochemical neuron (1T-OECN) enabled by a BBL-derived organic electrochemical memtransistor (OECmT) [1]. By tailoring electrolyte composition and driving conditions, the device achieves stable hysteretic switching with an on/off ratio of ~150 maintained over 2,000 cycles. The intrinsic electrochemical dynamics of the OECmT support rich neuronal functionalities without auxiliary circuitry, including threshold-triggered action potentials, tonic and phasic firing, bursting, spike-frequency adaptation, and nonlinear Boolean logic operations. With an active footprint of ~180 μm^2, the 1T-OECN supports integration densities exceeding 62,500 neurons cm^{-2} on flexible substrates. We further demonstrate tactile signal encoding via pressure sensors, pathway-like spike propagation across device arrays, and implementation of all six fundamental Boolean operations (AND, OR, XOR, NAND, NOR, XNOR), each realized within a single transistor. This minimalist, material-driven architecture establishes a scalable paradigm for organic neuromorphic hardware, combining bio-realistic spiking dynamics with high-density, mechanically compliant platforms suitable for next-generation implantable and biointegrated systems.

References

J. Ji, D. Gao, H. Y. Wu et al., Nat. Commun. 16, 4334 (2025)

Supramolecular Hybrid Hydrogels from Cellulose Nanofibrils and Fmoc-Diphenylalanine for Biomedical Applications

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This study examines supramolecular hybrid hydrogels composed of TEMPO-oxidized cellulose nanofibrils (CNF) and the self-assembling peptide Fmoc-diphenylalanine (Fmoc-FF). Hydrogels were synthesized by dispersing cellulose nanofibers in dimethyl sulfoxide, subsequently incorporating peptides at varying quantities, with gelation initiated by the addition of water. Rheological characterization, encompassing strain sweep, frequency sweep, steady shear, and recovery tests, was conducted to assess viscoelasticity, flow behavior, and structural dynamics. In comparison to the CNF control, the hybrid systems demonstrated markedly improved storage modulus (G′) and viscosity, with G′ regularly exceeding G″, thereby validating the establishment of resilient supramolecular networks. FE-SEM research demonstrated the transformation from a lamellar CNF structure to a compact three-dimensional fibrillar architecture following peptide incorporation. While the 0.05 g system showed greater stiffness but a more brittle response and quicker recovery after shear, the 0.09 g formulation created a more cohesive, entangled, dissipative network with higher complex viscosity. These results demonstrate that peptide concentration governs the balance between stiffness, connectivity, dissipation, and recovery in CNF/Fmoc-FF hydrogels, highlighting their potential for biomedical applications requiring tunable rheology and structural control.

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References
Caló, E.; Khutoryanskiy, V. V., Eur. Polym. J., 65, 252–267 (2015).

Alves, W.A. et al., Macromol. Chem. Phys., 220, 1900085 (2019).

Alves, W.A. et al., Biomed. Mater. Devices, 4, 1325-1362 (2026).

The impact of dynamic disorder on transport in doped semiconducting polymers

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It has recently been demonstrated that the strong coupling between electron and ion dynamics in polymeric organic mixed ionic-electronic conductors (OMIECs) causes significant dynamic disorder in the energy levels of localized carrier states in the intermediate timescale (5-500ps), fast enough to drive the charge transport and mitigate the effects of large static disorder in these materials [1]. We extend this investigation here to an expanded set of OMIEC polymers, employing an accelerated version of a scheme based on the combination of MD simulation and QM/MM calculations to treat the coupling of ion dynamics and polymer excess charge within a material [2]. The significant impact on the energy landscape of allowing excess charge to reorganise due to ionic motion in OMIECs is demonstrated, and the effects of backbone and side-chain chemistry, microstructure/swelling, and level of doping on the magnitude of site-energy fluctuations are investigated within this framework, allowing structure-property relationships to be defined. Furthermore, we show that charge carrier mobility in OMIEC polymers can be quantified using kinetic approaches parametrised directly from the MD-derived site-energies, explicitly mapping the microscopic origin of dynamic disorder to the macroscopic charge mobility and allowing direct comparison with experimental results.

Acknowledgements
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References
[1] C. Burke, A. Landi, A. Troisi, Mater. Horiz. 1 (21), 5313-5319 (2024)

[2] A. Landi, M. Reisjalili, J. D. Elliott, M. Matta, P. Carbone, A. Troisi, J. Mater. Chem. C 11, 8062-8073 (2023)

Water soluble emissive diradicals for quantum biosensing

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Electron spin states are attractive building blocks for quantum technologies, including quantum computing, where spin states function as qubits, and quantum sensing, where small environmental changes, such as chemical binding events, solvent polarity, local magnetic fields, pressure, or temperature, perturb the spin state in a detectable manner [1]. While solid-state platforms dominate current research, organic radicals offer a compelling molecular alternative: they are chemically tuneable, potentially biocompatible, and can be engineered with atomic-level precision. However, most organic radicals are non-emissive, restricting their investigation primarily to specialised magnetic resonance techniques. Recent advances in chlorinated triphenylmethyl (trityl) radicals have overcome this limitation, yielding air-stable, emissive radical species that permit direct optical interrogation of spin states [2]. Molecules containing two coupled radical units (diradicals) are particularly attractive in this context, as their singlet (antiparallel) and triplet (parallel) spin states can be distinguished with high contrast using fluorescence spectroscopy [3]. Here, we present a modular synthetic strategy for the preparation of emissive organic diradicals compatible with aqueous environments, achieved through the controlled introduction of solubilising substituents while preserving radical stability, emissive behaviour, and spin–spin coupling. Building on this platform, we further demonstrate post-synthetic functionalisation routes enabling the installation of reactive handles such as NHS esters and azides for bioconjugation. These chemically addressable, water-soluble emissive diradicals establish a foundation for targeted imaging and optically readable quantum biosensing in complex chemical and biological environments.

References

N. Aslam et al., Nat. Rev. Phys., 5, 157–169 (2023)

P. Murto & H. Bronstein, J. Mater. Chem. C, 10, 7368-7403 (2022)

R. Chowdhury et al., Nat. Chem., 17, 1410–1417 (2025).

3D-Printed Hollow Carbon-Paste Microneedle Electrodes as Electroactive Platforms for Future Immunosensing Applications

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Minimally invasive electrochemical platforms capable of accessing dermal interstitial fluid are important for point-of-care monitoring of clinically relevant biomarkers. Here, we report the fabrication and physicochemical characterization of a 3D-printed hollow microneedle carbon electrode as an electroactive platform for future biosensing and immunosensing applications. The device was produced by stereolithography and integrated hollow microneedles into a planar connector architecture inspired by screen-printed electrodes. Each microneedle had a height of 1.5 mm, outer diameter of 1.0 mm, and internal channel diameter of 0.57 mm, allowing carbon paste incorporation as a confined conductive phase. Optical and scanning electron microscopy confirmed the hollow geometry, open microchannels, and a continuous conductive pathway after filling. Mechanical compression assays showed nearly overlapping force–displacement profiles for electrodes with and without carbon paste, indicating preserved structural response. Insertion-mimicking assays demonstrated perforation of stacked polymeric layers. Oxygen plasma treatment increased wettability and modulated the electrode/electrolyte interface. Electrochemical measurements using $[Fe(CN)_6]^{3-/4-}$ and $[Ru(NH_3)_6]^{3+/2+}$ redox probes demonstrated improved accessibility, lower interfacial resistance, and enhanced conductive-phase connectivity after plasma activation. Ascorbic acid and dopamine oxidation were used as model reactions to evaluate analyte-dependent electroactivity, showing that plasma treatment selectively modulates the interfacial response according to redox mechanism and analyte charge. Overall, the platform combines mechanical robustness, insertion capability under model conditions, three-dimensional conductivity, and tunable interfacial electrochemistry, making it a promising transducer for future minimally invasive biosensing platforms, including antibody-based immunosensors for inflammatory biomarkers such as IL-6.

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References
Alves, W.A. et al., Biomed. Mater. Devices, 4, 1325-1362 (2026).

Alves, W.A., Braz. J. Anal. Chem. 13, 13-15 (2026).

Alves, W.A. et al., ACS Appl. Bio Mater. 9, 2419-2433 (2026).

Beer-Gated ZnO Transistors for Contamination Detection

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This research explores the development of electrolyte-gated transistors (EGTs) using spray-coated zinc oxide (ZnO) as a sensing platform to detect toxic contaminants, specifically ethylene glycol (EG) and diethylene glycol (DEG), in beer. These substances pose significant food safety risks, and traditional detection methods often require costly, centralized laboratory equipment. To address this, the study introduces a "sample-is-the-sensor" paradigm in which pretreated beer directly serves as the gate electrolyte. The fabrication involved a custom-built automated ultrasonic spray pyrolysis system to ensure high reproducibility and uniformity of the ZnO thin films. Because the natural acidity and carbonation of beer can degrade metal oxides, the samples underwent a pretreatment protocol involving pH neutralization and degassing. The study employed a randomized factorial design to evaluate how beer style (Pilsner vs. Weizenbier), contaminant type, and concentration affect electrical performance. Results showed that the devices operate at low voltages (below 1 V) with high drain currents. Statistical analysis (ANOVA) revealed that different electrical parameters respond to different factors: the threshold voltage is primarily influenced by the beer matrix's properties, while current hysteresis is more sensitive to the specific type and concentration of the glycol contaminant. The platform successfully detected contaminants at levels 5 times below the toxicity threshold, demonstrating its potential as a low-cost, portable, and rapid screening tool for food safety and quality control in the brewing industry.

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References

[1] Schep, L. J., Slaughter, R. J., Temple, W. A., & Beasley, D. M. G. (2009). Diethylene glycol poisoning. In Clinical Toxicology (Vol. 47, Issue 6, pp. 525–535). https://doi.org/10.1080/15563650903086444

[2] Kim, S. H., Hong, K., Xie, W., Lee, K. H., Zhang, S., Lodge, T. P., & Frisbie, C. D. (2013). Electrolyte-gated transistors for organic and printed electronics. In Advanced Materials (Vol. 25, Issue 13, pp. 1822–1846). https://doi.org/10.1002/adma.201202790

[3] Cramer, T., Campana, A., Leonardi, F., Casalini, S., Kyndiah, A., Murgia, M., & Biscarini, F. (2013). Water-gated organic field effect transistors-opportunities for biochemical sensing and extracellular signal transduction. In Journal of Materials Chemistry B (Vol. 1, Issue 31, pp. 3728–3741). Royal Society of Chemistry. https://doi.org/10.1039/c3tb20340a

Development of active packaging using a ternary blend of Poly(butylene adipate co-terephthalate), poly(lactic acid), and thermoplastic starch

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Approximately one-third of all food produced globally is lost or wasted each year, with microbial contamination being a major contributor to spoilage. Fatty foods, such as meats, cheeses, and processed products, are particularly vulnerable to oxidative deterioration and rancidity. To address the global problem of food waste, this proposal seeks to create sustainable and efficient active packaging materials, with an emphasis on fatty food items. The project will employ a ternary blend of commercially available compostable polymers, including poly(butylene adipate-co-terephthalate) (PBAT), poly(lactic acid) (PLA), and thermoplastic starch (TPS), and combine them with varying amounts of thymol, a natural antimicrobial and antioxidant compound that is derived from thyme essential oil. The resulting films' physicochemical and functional characteristics, such as their UV-blocking, antimicrobial, and antioxidant capacities, will be assessed in this study. Additionally, the incorporation of thymol into the blend matrix will be explored using industrial processing techniques such as extrusion and hot pressing to develop packaging able to extend the shelf life of fatty foods while reducing the environmental impact of conventional plastics. Furthermore, the release profile of thymol from the films into fatty food simulants will be assessed. This project is expected to provide processing conditions for PBAT/PLA/TPS blends that incorporate an appropriate amount of thymol to prevent microbial growth and oxidative spoilage, offering a sustainable solution for food preservation and safety.

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References
Q. Liang, P. A. Kilmartin and Q. Gao, Food Chem, 2025, 465, 142070

Effects of Different Concentrations Gadolinium and Yttrium doping on the Structural and Vibrational Properties of Molybdenum Trioxide with Potential application for Gas Sensing

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This study investigates the influence of gadolinium and yttrium doping on the structural and vibrational properties of molybdenum trioxide (MoO_3) as a function of dopant concentration, with emphasis on structure–property relationships relevant to functional applications. MoO_3 has attracted significant interest due to its versatile optical, electronic, and catalytic properties, while Raman spectroscopy provides a sensitive probe of its lattice dynamics and structural order [1]. Rare-earth doping has emerged as an effective route to tailor these properties; however, the role of dopant concentration in defect formation and lattice distortion remains insufficiently understood. Pure and doped MoO_3[2] crystals were synthesized via thermal decomposition of ammonium heptamolybdate tetrahydrate ($(NH_4)_6Mo_7O_{24}\cdot 4H_2O$). Gadolinium and yttrium were introduced using nitrate precursors at concentrations of 1%, 2%, and 3%. The precursor solutions were prepared in methyl alcohol, homogenized, and calcined at 450 ºC for 6 h. The resulting powders were characterized by Raman and FTIR spectroscopy at room temperature. Raman spectra exhibited characteristic Mo–O vibrational modes, while doped samples showed systematic band broadening, peak shifts, and intensity variations depending on dopant type and concentration. These features are attributed to lattice distortions and defect states induced by substitutional incorporation of rare-earth ions [3]. FTIR analysis confirmed these modifications, revealing shifts to lower wavenumbers and changes in band profiles associated with alterations in the local bonding environment. These modifications are directly linked to changes in electronic structure and surface reactivity, highlighting the potential of rare-earth-doped MoO_3 for gas sensing applications. This work provides insights into defect engineering strategies for tailoring oxide materials toward advanced functional applications.

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References
[1] Dieterle, M.; Weinberg, G.; Mestl, G. Raman spectroscopy of molybdenum oxides. Physical chemistry chemical physics: PCCP, v. 4, n. 5, p. 812–821, 2002

[2] Lima, C. D. A., et al. Co-doped α-MoO3 hierarchical microrods: Synthesis, structure and phonon properties. Ceramics international, v. 47, n. 19, p. 27778–27788, 2021.

[3] Martins, T. S.; Isolani, P. C. Terras raras: aplicações industriais e biológicas. Química nova, v. 28, n. 1, p. 111–117, 2005

Electrochemical detection of heavy metals using hybrid conjugated polymer/silver nanoparticle-based electrodes

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Nanostructured materials have attracted considerable attention in organic electronics and sensing technologies due to their high surface area, tunable physicochemical properties, and ability to promote efficient interfacial charge transfer [1]. Hybrid systems combining organic semiconducting nanoparticles with metallic nanostructures are particularly promising for the development of functional electrochemical sensing platforms [2,3]. In this work, conjugated polymer nanoparticles (CPN) based on a fluorene–thiophene copolymer were combined with silver nanoparticles (AgNP) to fabricate a hybrid nanostructured electrode for heavy metal detection. The material was assembled on biodegradable gPBAT films through a layer-by-layer approach, resulting in the architecture gPBAT(CPN:AgNP/PEI)6. Square-wave voltammetry (SWV) measurements revealed well-defined stripping peaks for Cd2+ and Cu2+ at distinct potentials, around −0.55 V and +0.10 V, respectively, with peak currents increasing as a function of metal ion concentration. The analytical response showed linear behavior in the concentration range from 0.1 to 2.1 mM, with correlation coefficients of $R^2 = 0.97$ for Cd2+ and $R^2 = 0.88$ for Cu2+. Recovery tests yielded values between 89-92% for Cd2+ and 89-100% for Cu2+, demonstrating suitable accuracy and reproducibility. The enhanced electrochemical response is attributed to the synergistic interaction between CPN and AgNP, which increases the electroactive surface area and facilitates charge transfer at the electrode/electrolyte interface. These results highlight the potential of hybrid organic–inorganic nanostructures as functional platforms for electrochemical sensing and environmental monitoring of heavy metals.

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References

S. Kang, et al., ACS Appl. Nano Mater., 5, 12 (2022)

C. M. Hangarter, et al., Nano Today, 8, 39 (2013)

G. Chen, et al., J. Mater. Chem. A, 13, 22365 (2025)

Electropolymerized poly(p-phenylenediamine) films for electrochemical detection of DNA nucleobases

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The development of functional materials for electrochemical biosensors has attracted increasing attention due to their tunable electronic structure and efficient interfacial charge-transfer properties. Conductive polymers obtained by electropolymerization are particularly attractive for electrode modification because they can form stable electroactive films that improve sensitivity, selectivity, and molecular recognition in electrochemical sensing platforms [1]. Among these materials, poly(p-phenylenediamine) (PpPD) stands out due to its π-conjugated back chain and the presence of amine functional groups, which facilitate electron transfer processes and promote interactions with biomolecules [2]. In this work, thin films of PpPD were electropolymerized onto graphite electrodes and investigated as functional interfaces for the electrochemical detection of DNA nucleobases. The polymeric coating was obtained by cyclic voltammetry electropolymerization of p-phenylenediamine, producing a conductive and chemically functionalized surface suitable for electrochemical sensing. The morphological characterization of the modified electrodes was performed by AFM, FTIR, XRD, and SEM. Electrochemical characterization was performed in a phosphate buffer solution containing adenine, cytosine, guanine, and thymine. The modified electrode exhibited well-defined oxidation responses that enabled electrochemical discrimination of the four nucleobases. Under individual detection conditions, oxidation potentials of 1.05 V, 1.38 V, 0.72 V, and 1.14 V were observed for adenine, cytosine, guanine, and thymine, respectively. In simultaneous detection experiments, distinct oxidation peaks were observed at 0.87 V, 1.22 V, 0.60 V, and 1.04 V. These results demonstrate that electropolymerized PpPD films provide an efficient conjugated electroactive interface capable of promoting enhanced interfacial charge transfer and enabling selective electrochemical biosensing of nucleic acid components.

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References

[1] Pan, Y.; Chen, J.; Li, H.; Zhang, Y. Recent Advances in Conductive Polymer-Based Electrochemical Sensors for Biomedical and Environmental Applications. Polymers 2024, 16, 1597. https://doi.org/10.3390/polym16111597

[2] Chen, G.; Li, X.; Wang, Y.; Zhang, H. Conjugated polymer nanoparticle-enhanced molecularly imprinted poly(o-phenylenediamine) electrochemical sensors for trace

detection. Journal of Materials Chemistry A 2025, 13. https://doi.org/10.1039/D5TA03236A

Eumelanin pigment-based doping for thermopower improvement in PEDOT:PSS blends

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Organic thermoelectric devices based on conducting polymers are promising for wearable and self-powered technologies, but improving electrical conductivity through conventional doping often reduces the Seebeck coefficient, limiting efficiency. Recent studies have shown that open-shell radical systems can enhance thermoelectric performance by increasing thermopower while maintaining charge transport. In this context, eumelanin, a natural and biocompatible pigment with an intrinsic stable radical population, mixed ionic/electronic conductivity, and semiconducting behavior, has emerged as a promising additive for conducting polymers. Previous work demonstrated that blending eumelanin with PEDOT:PSS modifies the polymer morphology and electrical properties, improving device performance. This study investigates the relationship between the Seebeck coefficient and the electron paramagnetic resonance (EPR) properties of eumelanin–PEDOT:PSS blends. The results show that the semiquinone moieties of eumelanin act as radical-active species that enhance thermopower. The pH-dependent semiquinone redox equilibrium, combined with the acidity of PEDOT:PSS, leads to a synergistic increase in radical concentration, which correlates with higher Seebeck coefficients. Based on EPR analysis and materials chemistry considerations, the authors propose that interactions between PEDOT radical cations and eumelanin radical anions are responsible for this effect. These findings demonstrate that eumelanin can act as a natural radical dopant capable of modulating the balance between conductivity and thermopower in PEDOT-based materials, opening new opportunities for sustainable, biocompatible thermoelectric systems and energy-conversion applications in organic electronics.

References

Ferraiuolo et. al. A synergistic radical concentration increase in eumelanin–PEDOT:PSS blends: mammalian pigment-based doping for thermopower improvement, Mater. Adv., 2024,5, 6967-6973

J. V. Paulin , A. Batagin-Neto and C. F. O. Graeff , J. Phys. Chem. B, 2019, 123 , 1248 —1255

J. V. Paulin , S. Bayram , C. F. O. Graeff and C. C. B. Bufon , ACS Appl. Bio Mater., 2023, 6 , 3633 —3637

Exploiting capacitive effects within a Saxitoxin aptamer-based biosensor

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Electrochemical Impedance Spectroscopy drives modern biosensing, but its potential is limited by equivalent electrical circuit (EEC) fitting. Furthermore, traditional charge transfer resistance calculations face physical ambiguities and require redox mediators, increasing complexity and toxic waste [1]. This work explores some electrical double-layer dynamics without preconceived circuit templates. We demonstrate that frequency-dependent parameters and relaxation time constants serve as robust sensing signals [2]. Using an aptamer-based biosensor for saxitoxin detection developed on screen-printed electrodes as a model system, we evaluated various non-faradaic approaches in a redox-free regime. The focus was to map intrinsic changes at the electrode-electrolyte interface during molecular recognition. Our results demonstrate that monitoring intrinsic dielectric shifts and double-layer perturbations provides a direct and sensitive metric for analysis. To validate the device's practical applicability, measurements were also successfully performed using environmental water samples collected directly from a lagoon, achieving a limit of detection in the 0.1 nmol. L^{-1} range. These capacitive approaches align with findings that alternative electrical parameters significantly enhance the accuracy of impedimetric sensors [3]. By isolating interfacial variations without toxic indicators, this methodology not only improves the accuracy of impedimetric platforms but also facilitates the development of high-performance, green, and label-free sensing technologies capable of trace-level detection in real-world scenarios.

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References

R. Patel et al., Bioelectrochemistry 153, 108492 (2023)

A. C. Lazanas and M. I. Prodromidis, ACS Measurement Science Au 3, 162 (2023)

R. S. Amorim et al., Results in Chemistry 7, 101314 (2024)

Halogen-Terminated Ti_3C_2 MXenes for Interface Engineering in Perovskite Solar Cells

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Surface termination engineering in MXenes has attracted significant attention as a versatile route to tune their electronic properties [1]. In particular, halogen functionalization offers an alternative pathway to modify surface chemistry and electronic structure [2], although its effects are still not fully understood. In this work, Ti_3C_2 MXenes with -Cl and -Br terminations were synthesized via molten salt etching, followed by delamination through ionic salt intercalation. Structural and chemical characterization using XRD, XPS, and electron microscopy confirmed successful synthesis, functionalization, and exfoliation of the materials. Density Functional Theory (DFT) calculations reveal that halogen terminations significantly alter the electronic structure and surface states of Ti_3C_2, highlighting their role in modulating interfacial energetics [3]. Owing to their metallic character and low optical absorption, these MXenes were further explored as interfacial modifiers. Experimentally, the materials were incorporated (1 vol%) into an IT-4F-based composite and applied at the electron transport layer (ETL). Optical characterization (UV–Vis and photoluminescence) shows enhanced quenching for MXene-containing ETLs compared to pristine IT-4F, indicating improved charge extraction and reduced recombination. Mesoscopic PSCs (FTO/c-TiO_2/m-TiO_2/perovskite/PEAI/PTAA/Au) based on $Cs_{0.15}FA_{0.78}Pb(I_{0.8}Br_{0.2})_3$ exhibit enhanced performance upon MXene incorporation, with Br-terminated Ti_3C_2 achieving a power conversion efficiency of 17.06%. These results demonstrate that halogen termination is an effective parameter for tuning MXene electronic properties, with direct implications for interfacial charge transport in optoelectronic devices.

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References

Xiao-Tong Jia, Hong-Wei Xing, Xing-Wang Cheng, Zhao-Hui Zhang, Qiang Wang, Jin-Zhao Zhou, Yang-Yu He, and Wen-Jun Li. Two-dimensional nanostructured ti3c2tx mxene for ceramic materials: Preparation and applications. Nanomaterials, 15(3), 2025. ISSN 2079-4991. doi: 10.3390/nano15030204. URL https://www.mdpi. com/2079-4991/15/3/204.

Mian Li, Xinliang Li, Guifang Qin, Kan Luo, Jun Lu, Youbing Li, Guojin Liang, Huang Zhaodong, Lars Hultman, Per Eklund, Per Persson, Shiyu Du, Zhifang Chai, Chunyi Zhi, and

Qing Huang. Halogenated mxenes with electrochemically active terminals for high performance zinc ion batteries, 06 2020.

Seyedeh Kazemi, Samuel Ogunkunle, Oscar Allen, William Wen, Alan Wee-Chung Liew, Shiwei Yin, and Yun Wang. Halogenation effect on physicochemical properties of ti3c2 mxenes. Journal of Physics: Materials, 6, 06 2023. doi: 10.1088/2515-7639/ acd8f3.

Hybrid PCL membranes incorporating Au and Pt nanoparticles produced by PLAL for tunable angiogenesis control

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Pulsed laser ablation in liquid (PLAL) has emerged as a sustainable approach for the synthesis of ligand-free metallic nanoparticles, in agreement with green chemistry principles [1]. When performed in water, the plasma–liquid interface promotes several chemical reactions; however, the role of dissolved CO_2 has been largely overlooked. In this work, we investigate the possibility of inducing the Carbon Dioxide Reduction Reaction (CO_2RR) during PLAL of gold and platinum targets in water, including control experiments with inert gases at the liquid interface [2]. This process leads to the formation of metal–organic nanocomposites and carbon monoxide–rich gold nanoparticles resulting from the interaction between reaction products and metallic nanoparticles [3]. Spectroscopic analysis revealed the presence of Au–CO species when nanoparticles were synthesized in water in equilibrium with air or CO_2, while this signal disappeared under argon atmosphere. Previous biological investigations demonstrated that the presence of CO at the nanoparticle surface modulates endothelial morphogenesis, enabling either pro- or anti-angiogenic responses. To explore their potential in regenerative biomaterials, the laser-synthesized nanoparticles were incorporated into biocompatible polycaprolactone (PCL) membranes to produce hybrid scaffolds. Mechanical and structural characterization revealed flexible membranes with porous morphology suitable for biological interfaces. The angiogenic response was evaluated using the CAM assay. Membranes incorporating nanoparticles synthesized under ambient atmosphere exhibited a strong pro-angiogenic effect, whereas those prepared under argon displayed anti-angiogenic behavior, demonstrating that the PLAL environment enables tunable angiogenesis control. These results highlight new opportunities for engineering multifunctional bioinspired biomaterials for tissue regeneration.

Acknowledgements
This work was supported by CNPq, FAPERJ, and CAPES.

References

[1] V. Amendola et al. Room-Temperature Laser Synthesis in Liquid of Oxide, Metal- Oxide Core-Shells, and Doped Oxide Nanoparticles. A Eur. J., pp. 9206–9242, 2020.

[2] Tahir et al., “Pulsed-Laser-Driven CO2 Reduction Reaction for the Control of the Photoluminescence Quantum Yield of Organometallic Gold Nanocomposites,” Small Sci., vol. 4, no. 7, Jul. 2024.

[3] A. Chillà et al., “Sparking angiogenesis by carbon monoxide-rich gold nanoparticles obtained by pulsed laser driven CO2 reduction reaction,” J. Nanobiotechnology, vol. 23, no. 1, p. 590, Aug. 2025.

Influence of mucins on the membrane interaction of conjugated nanopolymer

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Nature-inspired strategies offer valuable insights into how nanomaterials interface with complex biological systems. In this context, conjugated polymers such as poly(3-hexylthiophene) (P3HT) have emerged as promising components in bioinspired and biomimetic systems due to their unique attributes, including electrical conductivity, mechanical flexibility, and biocompatibility [1]. This study explores the interaction between mucins, which are the major structural proteins of mucosal surfaces [2], and P3HT nanoparticles, using Langmuir monolayers as a membrane model. These monolayers consist of DPPE and DOPE, phospholipids that constitute a large fraction of bacterial membranes [3]. The aim was to understand how mucins affect the behavior of nanostructured P3HT in biological environments, particularly in the context of biocidal devices and antimicrobial applications. Nanostructured P3HT was synthesized via nanoprecipitation, and its saturation concentration was set at 75 µg/mL. Subsequently, a ternary Langmuir film system containing lipids (DPPE or DOPE), mucins and P3HT nanoparticles was used to investigate the interactions among these components as models of microbial cell membranes. Binding parameters such as the maximum insertion pressure (MIP) and synergistic interactions were used to analyze the films by surface tensiometry. P3HT exhibits stronger interactions with DOPE than with DPPE monolayers, as indicated by MIP values of 26.46 and 39.61 for DPPE and DOPE, respectively, suggesting preferential interactions with unsaturated lipid chains (such as DOPE) over saturated ones (like DPPE). The addition of mucins to the subphase did not significantly alter surface pressure values, likely due to the large size of the protein compared to the other components. This work highlights the potential of conjugated nanomaterials for mucosal antimicrobial applications, contributing to the development of biointerfaces with applications in biosensing and biotechnology.

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References
DENG, HM. P3HT-PbS nanocomposites with mimicking enzyme as bi-enhancer for ultrasensitive photocathodic biosensor. Biosensors & bioelectronics, v. 197, p. 113806, 2022.

CORFIELD, A. P. Mucins: A biologically relevant glycan barrier in mucosal protection. Biochimica et Biophysica Acta (BBA) - General Subjects, v. 1850, p. 236-252, 2015.

EPAND, R. M., EPAND, R. F. Lipid domains in bacterial membranes and the action of antimicrobial agents. Biochimica et Biophysica Acta (BBA) - Biomembranes. v.1788, p. 289-290, 2009.

Laser Induced Periodic Surface Structures on Eutectic Gallium-Indium Based Composites for Tissue Engineering

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Liquid metals such as eutectic gallium-indium alloy (EGaIn) have recently been in the center of attention for soft and stretchable electronics development and intelligent biomaterial fabrication, due to their unique liquid-state properties, high thermal and electrical conductivity, stretchability, non-toxicity, biocompatibility and recyclability [1]. Focus of this work was preparation of homogenous composites of EGaIn nanodroplets dispersed in polystyrene (PS) with different ratios and their subsequent surface modification. The PS-EGaIn composite polymer films were manufactured by method of solvent casting of homogenous liquid-particles colloidal solutions in selected solvents, prepared by high energy ultrasonication. To further enhance composite properties, other conductive fillers such as carbon nanofibers were also added. The polymer composite surfaces were exposed to polarized KrF laser treatment, with the range of laser fluence between 8 and 14 mJ.cm-2 with number of laser pulses 3000 and 6000. The laser exposure leads to the formation of LIPSS, laser induced periodic surface structure with dimensions of wavy structure approximately between 200 and 450 nm. Polystyrene has previously exhibited the ability to either maintain high cytocompatibility or even enhance the cytocompatibility in comparison to tissue polystyrene and enhanced with LIPSS have exhibited the potential of cell guidance for tissue engineering [2]. The introduction of EGaIn particles onto periodic nanopattern formed by laser exposure influenced the periodic network's capacity for developing bioactive surfaces. Additionally, polymers volume enhanced with EGaIn can acquire limited self-healing capabilities, as ruptured conductive paths formed by liquid metal droplets can spontaneously reconnect due to the properties of EGaIn.

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References
[1] Zhao, Z.; Soni, S.; Lee, T.; Nijhuis, C. A.; Xiang, D., Adv. Mater. 35 (2023), 2203391.

[2] N. Slepičková Kasálková, V. Juřicová, S. Rimpelová et al., Polym. Deg. Stab. 221 (2024) 110667.

Light-Responsive Conjugated Polymer Thin Films: Optical Sensing and an Attract-and-Eliminate Strategy for Biomphalaria

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The development of functional organic materials that convert optical stimuli into measurable responses remains a key challenge in Organic Optoelectronics. Conjugated polymers are attractive for this purpose due to their π-conjugated backbones, tunable photophysical properties, and compatibility with low-cost sensing architectures [1]. Here, we report a light-responsive platform based on thin films of the conjugated polymer MEH-PPV used as disposable colorimetric sensors integrated with LED illumination systems. Under blue-light irradiation (~450 nm), MEH-PPV films undergo photodegradation, resulting in chromatic shifts, reduced effective conjugation length, and changes in optical absorption [2]. The films exhibit stable response for 8–11 h, enabling their use as low-cost optical dosimeters for real-time monitoring of blue-light radiance. Controlled illumination was applied to investigate light–matter interactions in freshwater snails of the genus Biomphalaria, which serve as intermediate hosts for Schistosomiasis. Structural analyses of laboratory- and field-derived shells revealed variations in thickness, porosity, and roughness that modulate optical transmittance (~67% and ~23% of incident RGB radiation, respectively), while maintaining transparency in the blue region. Phototaxis assays in snails showed a preferential attraction to blue light (~53%), with an average approximate rate of approximately 1 cm min^{-1}. In contrast, continuous exposure to controlled blue radiance (8.4 μW cm^{-2} nm^{-1}), monitored by the polymer dosimeter, induced stress and mortality after approximately 2.5 hours. These results demonstrate an integrated optoelectronic strategy combining radiance sensing, attraction, and light-induced stress, highlighting the potential of π-conjugated polymers for light-mediated environmental sensing and vector-control technologies [3].

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References
[1] A. J. Heeger and J. Roncali, Chem. Rev. 110, 668 (2010)

[2] Z. Fu and J. Yao, Nanotechnology 35, 325203 (2024)

[3] T. T. Tran and J.-H. Yun, Polymers 16, 2371 (2024)

Methylene Violet 3RAX for Photodynamic Therapy of Melanoma

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Although melanoma accounts for a smaller fraction of skin cancers, it is the most aggressive and lethal subtype, posing significant therapeutic challenges[1]. Photodynamic therapy (PDT) has emerged as a promising alternative to conventional treatments due to its minimally invasive nature[2]. In this study, we investigated the phenazine-derived photosensitizer methylene violet 3RAX (MV) in PDT against A375 and SH-4 melanoma cell lines using in vitro assays and Langmuir monolayer analysis. MV showed no intrinsic cytotoxicity; however, upon light activation, it induced a dose-dependent response. Flow cytometry revealed late apoptosis as the predominant cell death mechanism under irradiation. Based on these 2D results, future studies will employ 3D spheroid models to compare responses between monolayer and three-dimensional systems. Langmuir isotherms demonstrated MV adsorption onto lipid monolayers, particularly interacting with anionic lipids. Irradiation promoted monolayer material loss due to hydroperoxidation, leading to lipid chain disruption and membrane destabilization. Overall, these findings support MV as a promising photosensitizer for PDT, warranting further evaluation in more complex biological models toward therapeutic applications.

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References
[1] F. Hoffmann-La Roche Ltd., Things You May Not Know About Skin Cancer, 2020.

[2] M. Ochsner, “Photophysical and photobiological processes in photodynamic therapy of tumors,” J. Photochem. Photobiol. B Biol., 39(1), 1–18 (1997). https://doi.org/10.1016/S1011-1344(96)07428-3

Near-infrared activated gold nanostars for efficient photothermal therapy of colorectal cancer

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Colorectal cancer is one of the most prevalent and deadly cancers worldwide, what the search for more effective and less invasive treatments1,2. In this context, photothermal therapy (PTT) has emerged as a promising strategy, using photothermal agents to convert light into heat, inducing localized hyperthermia and cancer cell death. Gold nanostars are particularly suitable due to their tunable localized surface plasmon resonance (LSPR) in the near-infrared (NIR), enabling deeper tissue penetration and efficient heat generation. In this study, silica-coated gold nanostars (AuNS@SiO2) were synthesized and evaluated as photothermal agents for colorectal cancer. UV-Vis spectroscopy showed an LSPR band at 838 nm. DLS analysis indicated a hydrodynamic diameter of 165.7 ± 7.8 nm and a zeta potential of +32.6 ± 0.3 mV, confirming colloidal stability. TEM images confirmed the nanostar morphology with a final diameter of 125.36 ± 17.90 nm. Interactions with cell membrane models were studied using Langmuir monolayers of lipid extracts from Caco-2 and HT-29 cells. AuNS@SiO2 incorporation expanded π–A isotherms, while FTIR indicated preferential interaction with polar head groups. Stability assays under irradiation (810 nm) revealed distinct effects: Caco-2 monolayers showed reduced area, suggesting lipid degradation, whereas HT-29 showed increased area, likely due to lipid peroxidation. The photothermal effect was assessed via MTT assays. Cells were incubated with AuNS@SiO2 (1:1–1:10, medium:AuNS@SiO2 solution) and irradiated (810 nm, 168.54 J/cm2). Cytotoxicity was observed above 1:4 (Caco-2) and 1:6 (HT-29). At non-toxic concentrations, irradiation reduced viability from 94.1% to 63.1% (Caco-2) and from 81.0% to 58.2% (HT-29) These findings highlight the potential of AuNS@SiO2 as efficient NIR-responsive photothermal agents for colorectal cancer therapy.

Acknowledgements
FAPESP (22/02189-2, 23/07375-1, 23/16973-0, 24/11383-2)

References

1. F. Bray, M. Laversanne, H. Sung, J. Ferlay, R. L. Siegel, I. Soerjomataram, A. Jemal, CA: A Cancer Journal for Clinicians 2024, 3, 35.

2. P. Danpanichkul, Y. Pang, P. Tothanarungroj, D. Dejvajara, D. Kim, P. Saokhie, K. Suparan, M. D. Muthiah, K. Duangsonk, D. O. Bernal, R. N. Lui, K. Wijarnpreecha, G. K. Abou-Alfa, M. B. Wallance, L. R. Roberts, A. G. Singal, J. D. Yang, Cancer 2026, 1, 12.

Neuromorphic behavior in thin films of polythiophene derivatives

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The Neumann architecture is defined by the physical separation between processing and memory units. This spatial gap imposes intrinsic latency in the system, as it requires constant data movement between these distinct functional blocks. Based on that, materials with neuromorphic behavior are important due to their capacity to emulate the human brain's synaptic plasticity, defined by the possible alteration of connection strength during neural activity [1,2]. In this work, this behavior was studied in thin films of regioregular poly(3-hexylthiophene) and poly(3-octylthiophene) analyzing changes in current by light stimulation. Both polymers were dispersed in chloroform, and the solution was drop-casted onto gold interdigitated electrodes. Synaptic-like plasticity was evaluated through current versus time measurements with different times of light-on and a fixed time of light-off between the cycles. Also, conductivity changes were estimated by current versus voltage measurements. To the analysis, reversibility and response variation per cycle were calculated. Furthermore, measurements of two pulses of light were performed to emulate paired-pulse facilitation (PPF). In general, the current reached higher values compared to the previous cycle, showing their synaptic plasticity, while there was an average tendency for a decrease in the variation in response and a tendency of increase in reversibility. Also, the average conductivity of the films increased after the cycle's exposure, with the greatest increase occurring for the longest exposure time, reinforcing the plasticity of the films [3]. In the case of two pulses, PPF was emulated even for 80 seconds between the pulses, revealing the long-term memory retention of both films [2]. Therefore, despite the simplicity of drop casting technique, both films exhibited neuromorphic behavior.

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References
HE, Yongli, et al., Recent Progress on Emerging Transistor-Based Neuromorphic Devices, Advanced Intelligent Systems, 3, 2000210 (2021).

T. Serghiou, et al., Biodegradable and Bioinspired UV Light Recognition via Sustainable Synaptic Transistors for Artificial Intelligence Vision Systems, Advanced Intelligent Systems, e202501338 (2026).

DAI, Shilei et al., Light-Stimulated Synaptic Devices Utilizing Interfacial Effect of Organic Field-Effect Transistors, ACS Applied Materials & Interfaces, 10, 21472-21480, (2018).

Strain-modulated flexible bio-organic/graphene/pet sensors based on dna-curcumin biopolymer

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Metal-free, environmentally friendly, and cost-effective piezoelectric strain sensors are increasingly attractive for next-generation wearable and flexible electronics. In this study, we developed a flexible bio-organic piezoelectric strain sensor based on deoxyribonucleic acid (DNA)-curcumin biopolymer integrated with graphene/PET substrates and investigated its strain-dependent current-voltage behavior. The fabricated device exhibited stable operation under both compressive and tensile deformation, confirming its mechanical flexibility and electromechanical response. In particular, the sensor showed a high strain gauge factor of 407 at an applied compressive strain of -0.027%, which is about 8.67 times higher than that of conventional metal-based strain gauges. In addition, the device demonstrated a rapid electrical response under a compressive strain of -0.08%, indicating its suitability for dynamic strain monitoring. The enhanced sensing performance is attributed to the piezoelectric characteristics of the DNA-curcumin thin film and its effective coupling with the flexible graphene/PET platform. These results suggest that the proposed bio-organic/graphene/PET sensor is a promising candidate for environmentally safe, lightweight, and wearable motion sensing applications, offering high sensitivity and mechanical adaptability compared with previously reported flexible strain sensors[1].

References

X. Liao, Q. Liao, X. Yan, Q. Liang, H. Si, M. Li, H. Wu, S. Cao, Y. Zhang, Adv. Funct. Mater. 25, 2395 (2015)

Synergistic NIR-Activated Phototherapy Mediated by Gold Shell-Isolated Nanostars Conjugated to ICG

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The progression of leukemia is driven by the uncontrolled expansion of malignant myeloblasts, highlighting the need for therapies to eliminate cancer cells with minimal off-target effects[1]. In this context, photothermal (PTT) and photodynamic (PDT) therapies have emerged as minimally invasive, light-activated approaches. PTT converts light into heat, while PDT uses photosensitizers (PS) to generate reactive oxygen species (ROS), inducing oxidative damage and cell death. Nanostructured platforms are well suited for integrating these modalities due to their tunable optical properties and ability to incorporate PS[2], enabling enhanced therapeutic outcomes through synergistic effects. Herein, gold shell-isolated nanostars (AuNS@SiO_2) were conjugated with indocyanine green (ICG) and coated with an additional silica layer, forming AuNS@SiO_2-ICG-SiO_2. Near-infrared (NIR) activation enables deeper tissue penetration and spectral overlap between the AuNS@SiO_2 plasmon resonance and ICG absorption, allowing simultaneous PTT/PDT activation. The system was characterized by UV-Vis and fluorescence spectroscopies, DLS, zeta potential, TEM, and photothermal assays (810 nm, 28.09 mW/cm²). ICG incorporation and the second silica layer were confirmed by a red shift in the plasmonic absorption band (830 to 835 nm), an increase in hydrodynamic diameter (109.9 to 135.7 nm), and a higher zeta potential (40.76 to 44.19 mV). Additionally, time-resolved spectrofluorescence measurements over 60 min revealed improved photostability of ICG within the silica layers. ICG conjugation also enhanced the photothermal response (15.4 to 18.2°C). Flow cytometry *in vitro* assays with HL-60 cells revealed time-dependent nanoparticle uptake, (photo)toxicity, intracellular ROS generation, and cell death pathways. Upon NIR irradiation, the nanoplatform predominantly induced late apoptosis at 1:4 and 1:6 ratios, highlighting its potential as a synergistic phototherapeutic platform for acute myeloid leukemia.

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References

1. H. Döhner, et al. Blood 2017, v. 129, n. 4, p. 424–447

2. M. Overchuk, et al. ACS Nano 2023, v. 17, n. 9, p. 7979–8003

Targeted Photodynamic–Photothermal Nanoplatform for Improved Melanoma Treatment

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Cancer remains a major global health concern, with skin cancer representing a significant proportion of diagnosed cases. Minimally invasive approaches such as photothermal therapy (PTT) and photodynamic therapy (PDT) have emerged as promising alternatives due to their selective and localized effects. [1] Photosensitizers (PS) generate reactive oxygen species (ROS) upon light activation, triggering oxidative stress-mediated cell death, while metallic nanoparticles induce hyperthermia under irradiation. The combination of PDT and PTT may enhance therapeutic efficacy through complementary mechanisms. In this study, silica-coated gold nanoparticles (AuSHINs) were conjugated with the photosensitizer Methylene Violet 3RAX (MV), followed by the deposition of a secondary silica layer (AuSHINs@MV@). Physicochemical characterization by UV–Vis spectroscopy, dynamic light scattering (DLS), zeta potential measurements, and transmission electron microscopy (TEM) confirmed monodispersity and a progressive increase in particle size after coating and conjugation. Cellular interactions were evaluated by confocal fluorescence microscopy using DAPI (nuclear staining), WGA-Alexa 488 (membrane labeling), and intrinsic PS fluorescence. Free MV was efficiently internalized, whereas AuSHINs@MV@ predominantly localized near the cell membrane after 2 h incubation. Although no evident morphological alterations were observed following irradiation, in vitro assays demonstrated a significant reduction in melanoma cell viability for AuSHINs@MV@ compared to free MV. The cytotoxic effect was incubation-dependent, decreasing viability to below 50% at 1 x1012 AuSHINs@MV@/mL after 2 h incubation and irradiation. Flow cytometry analysis indicated predominantly necrotic cell death. These findings confirm the successful synthesis and functionalization of the nanostructures and highlight their potential as a combined PDT/PTT platform for melanoma treatment.

Acknowledgements
FAPESP (2021/14500-1, 2024/05366-8, 2022/02189-2)

References
[1] Wang N, Zhao Z, Lv Y, et al. Gold nanorod-photosensitizer conjugate with extracellular pH-driven tumor targeting ability for photothermal/photodynamic therapy. Nano Res. 2014;7(9):1291-1301. doi:10.1007/s12274-014-0493-0

Ultrasensitive microRNA Biosensing Through Reduced Graphene Oxide Electrolyte Gated Transistors with Machine Learning

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Reduced graphene oxide (rGO) is a two-dimensional material widely used in various technological applications due to its tunable electrical conductivity and the presence of oxygen-containing functional groups [1]. These characteristics are desirable for developing new electronic sensors and biosensors, where (bio)chemical receptors can be grafted on the rGO flakes to support the recognition of target analytes. By employing rGO as an active layer in electrolyte-gated transistors (EGTs), highly sensitive, selective, and efficient chemical sensors and biosensors can be obtained [2]. Here, we report an ultrasensitive and selective biosensor that combines DNA-functionalized rGO, EGTs, and machine learning (ML) for ultrasensitive and selective miRNA detection. Our strategy focuses on the miR34 family, namely miR-34a, miR-34b, and miR-34c, which are associated with neurological disorders and present potential for animal health diagnostics. A covalent functionalization approach was explored using EDC/NHS. Ethanolamine was employed as a blocking agent to prevent nonspecific binding at the device surface. The EGT transfer curves were obtained by measuring the source-drain current (IDS) as a function of the gate-source voltage (VGS), ranging from +0.3 to -0.1 V, while maintaining a constant source-drain voltage (VDS) at 0.1 V. The biosensor reliably discriminated perfectly matched from mismatched sequences over a dynamic range of 0.1–1,000 amol L^{-1}, achieving an ultralow limit of detection of 0.098 amol L^{-1}. ML provided multidimensional signal analysis of the EGT transfer curve and the extraction of physically meaningful relationships from high-dimensional data. This work represents a significant advance in portable diagnostic devices for the ultrasensitive and highly selective biosensing of miRNAs.

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References
Park, D. et al., Biosens. Bioelectron. 167, 112505 (2020).

Furlan de Oliveira, R, et al. Advanced Functional Materials, 2019. 29(46): p. 1905375.

Electronic Structure of Halide Perovskite Materials for Energy Conversion Applications

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Halide perovskites are a novel class of thin-film semiconductors that have revolutionized the field of photovoltaics and now reach efficiencies comparable to state-of-the-art silicon solar cells. Their remarkable defect tolerance, solution-based processability, and tunable band gap make them highly promising materials for next-generation optoelectronic and energy-conversion technologies.

This talk will discuss the origins of the exceptional semiconducting properties of halide perovskites with a focus on their unique and tunable electronic structure. To address this, we employ in our labs a combination of photoelectron spectroscopy techniques, including ultraviolet photoelectron spectroscopy (UPS), inverse photoelectron spectroscopy (IPES), and reflection electron energy loss spectroscopy (REELS), which together allow us to probe both occupied and unoccupied electronic states.

Using these methods, we investigate how atomic structure, lattice distortions, and bonding interactions influence the valence and conduction band density of states in both lead- and tin-based perovskites. In addition, I will discuss our recent work on reduced-dimensionality perovskites, where two-dimensional (2D) layers formed by organic spacer cations are used to modify surfaces and interfaces. Systematic studies with alkylammonium spacers of varying chain length reveal how interlayer spacing and structural distortions influence the electronic and optical properties of these materials.

Overall, these results provide insight into how composition and dimensionality affect band structure and interface energetics in halide perovskites, contributing to a deeper understanding of the fundamental electronic properties that govern their performance in optoelectronic and energy-related applications.

Generating Charges in Organic Photovoltaic Systems

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Organic Solar Cells, Spectroscopy, Charge Generation

The objective of my group is to use ultrafast spectroscopic techniques, such as transient absorption (TA), electro-modulated differential absorption (EDA) or time-domain terahertz (TD-THz) spectroscopy, to investigate charge carriers in organic photovoltaic (OPV) materials. While femtosecond TA measurements bring insights to the nature and evolution of the photoexcited species, EDA reveals the charge separation dynamics, and we use TD-THz spectroscopy to gain information about the nanoscale charge transport. In this talk, I will present an overview of our results obtained in recent years about the different steps of charge generation in OPVs. After presenting our experimental techniques, I will show results about charge generation in highly efficient solar cell materials based on organic polymer:fullerene and polymer:non-fullerene blends with negligible driving force for interfacial charge transfer, as well as on evaporated dilute solar cells. I will discuss how charge generation and recombination processes depend on parameters such as the charge transfer driving force, the short-range charge mobility and the morphology. The combination of our results allows to visualize all relevant processes that lead to efficient charge extraction in full devices.

Light as a tool in Energy and environment. Perspectives and discussions

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Keywords: Electrocatalysis, Plasmonics, nanomaterials

Nanoelectrochemistry brings the advantage of using nanoparticles with unique properties when compared to their bulk counterparts. Among those properties, in the case of metals, there is the localized surface plasmon resonance (LSPR), which gives rise to valuable physical effects such as hot-carrier generation and local heating effect. However, not every metal presents the LSPR on the visible range of the spectrum and, thus, requires specific and costly apparatus to optimize LSPR outcomes. However, it makes a valuable challenge to tune the LSPR extinction band toward the visible spectrum through the rational design of nanoparticles. One strategy is to combine different metals with catalytic and plasmonic properties in hybrid nanostructures, allowing an improved energy harvesting and catalytic activity toward electrochemical reactions upon excitation at the visible spectrum. A systematic study of the synthesis of different bimetallic or hybrid semiconductor/metallic nanoestructures is presented. The materials exhibited the LSPR excitation in different regions of the visible range of the spectrum depending on their composition, size or geometry. Distinct electrochemical reactions were chosen to evaluate the LSPR excitation impact on the catalyst's activity and/or selectivity showing that each electrochemical reaction was affected differently by the LSPR excitation. This work provides a concise overview of the fundamental principles of LSPR; the mechanism of plasmon enhanced electrocatalysis; recent progress in plasmon-mediated electrocatalysis for the detection of analytes and the synthesis of chemicals such us green ammonia and urea. This idea is also to shed light on the areas where major advancements are required to further improve the field of plasmon-mediated electrocatalysis to achieve a major paradigm shift toward a sustainable future.

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Navigating the dopant:host phase space to rationalize chemical doping of semiconducting polymers: A journey from excitons, polarons to trions

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Keywords: polymer semiconductors, chemical doping, trions

The utilization of chemical doping in polymer semiconductors is imperative for controlling charge transport in this interesting materials class. However, polymer-dopant blend compositions of highest electrical conductivities are generally identified by empirical means, despite the strong correlation of performance with molecular interactions, thermodynamic stability, and solid-state structure. Here, we demonstrate that the temperature-composition phase space provides a unifying framework that encompasses these interdependencies and reveals the physico-chemical basis for rationalizing chemical doping. Specifically, eutectic phase-diagram features manifest as thermodynamic imprints of strong interactions between the semiconductor and the dopant, reflecting the balance between charge transfer and molecular stacking frustration and suppressed crystallization/vitrification that dictate molecular mixing as well as phase stability. Our phase-space description, thus, enables prediction of charge transport across temperatures and compositions, unambiguously representing an advance on current post-hoc optimization procedures and providing transferable, a priori design principles to realize efficient chemical doping in semiconducting polymers from the outset. Moreover, mapping this phase space clarifies the structural regimes where electronic species such as polarons and excitons coexist and interact, creating conditions favorable for trion formation and allowing us to establish trions as general, intrinsic species in doped polymer semiconductors, rooted in the same thermodynamic and structural principles that govern phase behavior.

Rational Design and Operando Understanding of Catalytic Sites for Renewable Energy and Sustainable Carbon Conversion

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The transition toward a sustainable energy future requires catalytic processes that efficiently convert renewable feedstock while mitigating carbon emissions. In this context, understanding the nature of catalytically active sites and their evolution under reaction conditions is essential for the rational design of next-generation catalysts. Our research combines nanoscience, heterogeneous catalysis, and operando characterization to establish structure–property relationships in catalytic materials relevant to renewable energy and sustainability. We investigate well-defined catalytic systems ranging from supported nanoparticles to single-atom catalysts and multicomponent oxides [1–3]. Strategies based on preformed nanoparticles, heterogenized coordination complexes, and high-entropy oxides enable control of metal dispersion, metal–support interactions, reducibility, and surface composition. These platforms allow us to probe how dynamic structural transformations influence catalytic performance. Emphasis is placed on CO_2 hydrogenation and hydrodeoxygenation (HDO) of biomass-derived molecules. In CO_2 conversion, the interplay between metallic and oxidized surface sites governs reaction pathways and selectivity toward CO, methanol, or methane [2]. In HDO, the balance between redox, acidic, and metallic functionalities controls C–O bond activation and the selective upgrading of oxygenated compounds into fuels and value-added chemicals [3]. A central aspect of this work is the use of advanced characterization techniques, including near-ambient-pressure X-ray photoelectron spectroscopy (NAP-XPS), in situ X-ray diffraction (XRD), and diffuse reflectance infrared Fourier transform spectroscopy (DRIFTS), including modulation excitation phase-sensitive detection (ME-PSD-DRIFTS), to monitor catalysts under working conditions. By correlating catalyst evolution with catalytic performance, we aim to identify descriptors that guide the rational design of efficient and sustainable catalytic materials for future energy technologies

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[1] Destro, P.; Kokumai, T. M.; Scarpellini, A.; Pasquale, L.; Manna, L.; Colombo, M.; Zanchet, D. *ACS Catal. 8* (2), 1031–1037 (2018).

[2] Sousa, L. S.; Bertuzzi, A.; Rodrigues Fiuza, T. E.; Leite, E. R.; Benito, P.; Ferri, D.; Zanchet, D.; Beale, A. M. Identification of Transient Intermediates and Active Species in Atomic CZA Catalysts for CO2 Hydrogenation to Methanol. *J. Am. Chem. Soc.*, *147* (47), 43295–43316 (2025).

[3] Strapasson, G. B.; Sousa, L. S.; Báfero, G. B.; Leite, D. S.; Moreno, B. D.; Rodella, C. B.; Zanchet, D. Acidity Modulation of Pt-Supported Catalyst Enhances CO Bond Cleavage over Acetone Hydrodeoxygenation. *Appl. Catal. B Environ.*, *335*, 122863 (2023).

Showcasing multitasking: multiparametric biosensing examples using PEDOT:PSS devices

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Conducting polymers, specifically PEDOT:PSS, have been widely used for interfacing with biology in many form factors. Optical transparency of thin film devices, combined with electroactive properties can be used to great advantage in interrogating biological function. In the case of diagnostics, for example, for detection of pathogens or cancerous cells, the combination of optical and electronic monitoring can be highly advantageous in achieving quantitative (electrical) readouts, while simultaneously allowing validation (optical). In this presentation I will showcase our efforts in integrating supported lipid bilayers (SLBs) with membranes extracted from live cells, used for quantifying virus entry and screening of antivirals. Here, optical transparency allows confirmation of bilayer functionality before measurement. A second example is the capture of specific cells of cancerous origin on conducting polymer composite devices, where they can be observed optically and quantified electrically, before being released for downstream analysis. A third example showcases the sensing of analytes from complex in vitro models of tissues and organs. These examples highlight the multiparametric data that can be derived from devices designed to interface intimately with biological systems.

Sn/Pb perovskites challenges and opportunities for photovoltaics

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Keywords: metal halide perovskites, solar cells, Sn-Pb perovkites

Mixed Tin/Lead (Sn/Pb) perovskites have the potential to achieve higher performances in single junction solar cells than Pb-based compounds. Nowadays, the most used hole transport layer (HTL) for Sn/Pb based perovskite solar cells is PEDOT: PSS, even if there are many doubts on a possible detrimental role of this conductive polymer on th performance e long-term stability of the active layer.

Recently, we have shown that self-assembled monolayer [2-(3, 6-dibromo-9H-carbazol-9-yl) ethyl] phosphonic acid (Br-2PACz) can have great advantages when used as HTL of solar cells of active layer $Cs_{0.25}FA_{0.75}Sn_{0.5}Pb_{0.5}I_3$ [1]. Several factors seem to determine the increased perfomance respect to devices using PEDOT: PSS as HTL, the perovskite layer deposited on SAMs show an higher crystallinity, with reduced pinhole density and larger grains but also a reduced defect density at the burried interface. In my presentation I will show devices above 25% efficiency combining this HTL and a proper surface passivation.

References:

[1] M. Pitaro, J. Sebastian Alonso, L. Di Mario, D. Garcia Romero, K. Tran, T. Zaharia, M. B. Johansson, E. M. J. Johansson, M. A. Loi, *J. Mater. Chem. A*, **11**, 11755 (2023).

Gate-Driven Edible OECTs for Sustainable and Low-Power Gastrointestinal pH Sensing

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Monitoring pH variations along the gastrointestinal (GI) tract is essential for diagnosing disorders such as reflux, peptic ulcers, malabsorption syndromes, and inflammatory bowel disease. Conventional methods, including endoscopy and catheter-based probes, are invasive and unsuitable for frequent monitoring. Wireless ingestible capsules are less invasive, but still rely on rigid, non-edible components, raising concerns about retention, retrieval, and electronic waste. Edible electronics offers a sustainable route toward safe, transient, and low-complexity biomedical devices. Here, we present an edible organic electrochemical transistor (OECT) platform for GI pH sensing, based on inkjet-printed gold source/drain electrodes transferred onto ethyl cellulose, with copper(II) phthalocyanine (CuPc) as the semiconducting channel. A coiled platinum electrode is used as a model external gate to clarify the sensing mechanism. The transistor was characterized in buffers spanning pH 2.5–11 under low-voltage operation below 1 V. Transfer curves show systematic threshold-voltage shifts with a sensitivity of approximately 50 mV pH−1. Ag/AgCl reference-gated measurements show that the CuPc channel is not intrinsically pH-sensitive in the investigated gate-voltage window. Open-circuit-potential measurements reveal that the response originates from electrochemical potential shifts at the gate–electrolyte interface, which are transduced by the OECT into amplified drain-current modulation. Our work clarifies the sensing mechanism of CuPc-based edible OECTs and highlights the potential of transistor architectures for simplified edible chemical sensing. By avoiding conventional reference electrodes, exploiting intrinsic amplification, and using a direct-exposure geometry compatible with miniaturization, this platform represents a step toward safe, low-complexity, and sustainable edible devices for gastrointestinal pH monitoring.

References

[1] A. S. Sharova, F. Melloni, G. Lanzani, C. J. Bettinger, and M. Caironi, “Edible Electronics: The Vision and the Challenge,” Adv Mater Technol, vol. 6, no. 2, p. 2000757, Feb. 2021, doi: https://doi.org/10.1002/admt.202000757.

[2] C. Cheng et al., “A wireless, ingestible pH sensing capsule system based on iridium oxide for monitoring gastrointestinal health,” Sens Actuators B Chem, vol. 349, p. 130781, 2021, doi: https://doi.org/10.1016/j.snb.2021.130781.

Photoelectrocatalytic Study of Electrodeposited Nickel Oxide Films for Glycerol Oxidation

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Current environmental challenges highlight the need for clean and sustainable energy sources to replace fossil fuels. In this context, a promising approach to green hydrogen (H_2) production is water electrolysis, which occurs via the H_2 evolution reaction and the oxygen evolution reaction (OER). However, replacing the OER with the glycerol oxidation reaction (GOR) can substantially reduce overall cell potential [1]. Glycerol (GLY) is an attractive feedstock as a low-cost biodiesel byproduct, with high availability in countries such as Brazil. Among the transition metals investigated for this purpose, Ni-based materials have exhibited a remarkable performance. In particular, nickel oxide (NiOx) is a semiconductive material capable of generating e^-/h^+ pairs under UV irradiation, significantly improving its electrocatalytic activity [2]. In this work, NiOx films obtained through a pulsed electrodeposition technique [3] coupled with controlled annealing were investigated as photoelectrocatalysts under prolonged GOR cycling. The materials were immersed in a 0.1 mol L^{-1} NaOH/GLY solution and evaluated under dark and illuminated conditions using a UV light source (370 nm) over 2000 cyclic voltammetry (CV) cycles from 0.1 to 0.8 V at 100 mV s^{-1} and chronoamperometry (CA) at 0.5 V for 2 h under stirring. Results showed that illumination improved the electrochemical stability of the NiOx films and shifted the GLY E_{onset} to lower potentials, resulting in a current retention of 34% between the 2nd and 2000th cycles, compared with 23% under dark conditions. In addition, light-assisted CA exhibited 8% higher current retention than CA performed in the dark. Furthermore, 3 CV cycles at 20 mV s^{-1} conducted before and after all measurements revealed the preservation of active Ni species and overall film stability. These findings reveal that enhancing the semiconducting properties of NiOx though UV irradiation offers a viable and stable pathway for sustainable H_2 production.

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References
Xavier F. et al. International Journal Of Hydrogen Energy, 48, 31091-31100 (2023)

J. Wang et al. Angewandte Chemie International Edition, 65, (2026)

Qing S. et al. Materials Research Bulletin, 114, 10-17 (2019)

Use of metal alloys to reduce instability in perovskite solar cells

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Despite the rapid increase in the efficiency of perovskite solar cells (PSCs), these devices still present serious stability issues. In PSCs, the choice of metal used as electrical contact can also reduce the stability and lifespan of the devices, as discussed in recent experimental [1] and theoretical [2,3] works. Here, we investigated the stability of Cu:Ni metal alloys in PSCs. For that, alloys with different Cu:Ni ratios were electrodeposited using an electrochemical cell composed of glass-FTO/Ni-P as the working electrode and a Ti/Pt mesh as the counter electrode, immersed in electrochemical baths containing different proportions of NiCl2, CuSO4 and sodium citrate. Next, the stability of the alloys was evaluated at each stage of the device manufacturing process (standard cleaning, UV-ozone treatment and heat treatment), as well as upon their interaction with perovskite films of MAPbI3 or CsFAMAPbI3, after accelerated degradation tests. The results showed that heat treatment promotes the greatest reduction in sheet resistance (Rs) for all alloy compositions, indicating improved metallic connectivity of the films. Alloys with higher Ni content showed the lowest Rs values and greater stability against cleaning, UV-ozone treatment and heat treatment steps, while Cu-rich alloys exhibited higher Rs values and greater susceptibility to oxidation, as evidenced by EDS data. The evaluation of stability of these alloys when in contact with perovskite films after accelerated degradation tests revealed that alloys with higher Ni content were more stable, maintaining surface integrity and showing less evidence of corrosion or ionic diffusion. Cu-rich alloys, on the other hand, exhibited morphological changes, including degraded regions, evidence of corrosion points and possible reactions with halides released by the perovskite. The results highlight the need for fine-tuning the composition of the electrical contact metal in the search for PSCs with improved stability.

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References

[1] J. M. C. da Silva Filho, A. de Morais, R. R. Cesar, et al., Sol. Energy Mater. Sol. Cells, 276, 113043, (2024).

[2] I. C. Ribeiro, A. de Morais, L. G. Chagas, et al., J. Phys. Chem. C, 129, 19925 (2025).

[3] L. G. Chagas, A. de Morais, I. C. Ribeiro, et al., ACS Omega, 10, 60886 (2025).

WiRES Round Table Discussion

The Role of Women in Renewable Energy and Sustainability

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Round Table Topics

- Benefits of female leadership
- Women role models
- Balance between male and female responses to challenges and risks
- Making scientific research an inclusive world
- Male networking versus female solo-working
- The role of education and importance of leaning
- Mentoring and career development