IPOE 2026
Bologna Italy

VOLTERA BIOAGE advanced electronics Park SYSTEMS Gambetti

Day 1

Monday, 14th September

09:00 – 10:30 **Registration & Welcome Coffee**

10:30 – 11:00 **Conference Opening & Welcome Speech**
(University of Bologna)

Charge Trapping and Transport Mechanisms

Chair: TBA

11:00 – 11:30 **Modelling materials with mixed ionic-electronic transport: from brute force to reduced models**
Alessandro Troisi *et al.* *(Invited Talk - Univ. of Liverpool)*

11:30 – 11:45 **Ultra-Steep Switching and Trap-Minimized Interfacial Carrier Transport in Highly Layered Crystalline Organic Semiconductors**
Tatsuo Hasegawa *et al.* *(University of Tokyo)*

11:45 – 12:00 **Unraveling Exciton Transport and Self-Trapping in Conjugated Polymers**
Llinersy Uranga-Pina *et al.* *(CY Cergy Paris Université)*

12:00 – 12:15 **Phase behavior and electrical transport in DBTTF:HATCN donor–acceptor mixtures**
Andreas Opitz *et al.* *(Humboldt-Universität zu Berlin, Germany)*

12:15 – 12:30 **Investigation of transport in OECTs with Electrochemical Strain Wave Microscopy**
Filippo Bonafè *et al.* *(University of Bologna)*

12:30 – 14:00 **Lunch Break**

Molecular Modelling and Fundamental Mechanisms

Chair: TBA

14:00 – 14:30 **Understanding thermal transport in complex materials like organic semiconductors and metal-organic frameworks**
Egbert Zojer *et al.* *(Invited Talk - Institute of Solid State Physics, Graz University of Technology)*

14:30 – 14:45 **Universal free-energy scaling of quantum efficiency controlled by acceptor end group strength in organic solar cells**
Denis Andrienko *et al.* *(King Abdullah University of Science and Technology, Saudi Arabia)*

14:45 – 15:00 **Flipping the Rules: From Inverted Singlet-Triplet Gaps to Diradical Switches**
Francesco Di Maiolo *et al.* *(University of Parma)*

15:15 – 15:45 **Coffee Break**

Operation Mechanisms in Organic Devices

Chair: TBA

15:45 – 16:15 **Molecular Control of Polaron Formation and Transport in Organic Electrochemical Devices**
Ji-Seon Kim *(Invited Talk - University of Oxford, United Kingdom)*

16:15 – 16:30 **Tailoring Curcuminoid Synthesis for Surface-Patterned Optical Sensors and Sublimated Crystalline Electronic Frameworks**
Núria Aliaga-Alcalde *et al.* *(ICREA - Institució Catalana de Recerca i Estudis Avançats)*

16:30 – 16:45 **Co-Crystallization and Charge-Transfer Complex formation in Thin Films: a strategy for NIR Sensing Applications**
Georgios Atsas *et al.* *(Insituto de Ciencia de Materiales de Barcelona (ICMAB-CSIC))*

16:45 – 17:00 **All-organic lasers with efficient near-infrared emission**
María A. Díaz-García *et al.* *(Physics Department, University of Alicante, Spain)*

17:00 – 17:30 **Poster Pitches**
(3 minutes presentations of posters)

17:30 – 19:00 **Poster Session & Aperitivo**

Day 2 — Tuesday, 15th September

2D Materials, Perovskites and MOFs

Chair: TBA

09:00 – 09:30 **Multilayered perovskite heterostructures for photovoltaic applications**
Jacky Even *et al.* *(Invited Talk - Univ. Rennes, INSA Rennes, CNRS)*

09:30 – 09:45 **Flexible and High-Performance Perovskite-Polymer Composites for Dual X-Ray and Proton Direct Detection**
Andrea Ciavatti *et al.* *(University of Bologna)*

09:45 – 10:00 **Hybrid 2D Perovskite Thin Films as a tunable platform for Fast and Thermal Neutron Direct Detection**
Ilaria Fratelli *et al.* *(University of Bologna)*

10:00 – 10:15 **All-Solution-Processed Perovskite Light-Emitting Transistors Enabled by Fully Organic Architecture**
Kelment Zahoaliaj *et al.* *(ISMN - CNR, Bologna)*

10:15 – 10:30 **Weak exciton–phonon coupling in two-dimensional perovskite thin films for high-performance UV photodetection**
Elisabetta Colantoni *et al.* *(University of Bologna)*

10:30 – 11:00 **Coffee Break**

Materials for Interface Engineering

Chair: TBA

11:00 – 11:30 **Printable Electronics enabled by Supramolecular 2D Material Inks**
Cinzia Casiraghi *(Invited Talk - Department of chemistry, University of Manchester, UK)*

11:30 – 11:45 **Controlling Polymorphism in Organic Semiconductor Thin Films via Substrate Selection**
Marco Terruzzi *et al.* *(University of Milano-Bicocca, Department of Materials Science)*

11:45 – 12:00 **Operando Demonstration of Polymorphism–Performance Correlation in C8O-BTBT-OC8 OFETs**
Esther Barrena *et al.* *(Insituto de Ciencia de Materiales de Barcelona (ICMAB-CSIC))*

12:00 – 12:15 **Controlling Monolayer–Bilayer Transitions in Ph-BTBT-Cn Thin Films via Thermal Annealing and Molecular Mixing**
Alexandra Harbuzaru *et al.* *(Insituto de Ciencia de Materiales de Barcelona (ICMAB-CSIC))*

12:15 – 12:30 **Alkyl Chain Length Controls Polar Phases Stability in Asymmetric BTBT Thin Films**
Alba Cazorla *et al.* *(Insituto de Ciencia de Materiales de Barcelona (ICMAB-CSIC))*

12:30 – 14:00 Lunch Break

Hybrid, Organic and Inorganic Interfaces

Chair: TBA

14:00 – 14:30 **Galvanic Molecular Intercalation for Hybrid 2D Electronics**
Marco Gobbi *et al.* *(Invited Talk - Centro de Física de Materiales, CSIC-EHU, San Sebastián, Spain)*

14:30 – 14:45 **Self-assembled pentacene on monolayer WS_2: a bottom-up route to a type-II organic/TMD heterostructure**
Michele Capra *et al.* *(Technical University Dortmund)*

14:45 – 15:00 **Graphene-Metal interfaces: correlating structural and electrical characterization with defects and doping in Raman as a function of contact resistance**
Alessandro Kovtun *et al.* *(CNR, Bologna)*

15:00 – 15:15 **Critical role of polymer gate dielectrics on the charge carrier transport in perovskite field-effect transistors**
Tomasz Marszalek *et al.* *(Lodz University of Technology/MPI for Polymer Research, Germany)*

15:15 – 16:00 Coffee Break

Organic & Hybrid Sensors and Devices 1

Chair: TBA

16:00 – 16:30 **Electrolyte-gated organic field-effect transistors for point-of-care sensing**
M. Mas-Torrent *et al.* *(Invited Talk - Institut de Ciencia de Materials de Barcelona (ICMAB-CSIC))*

16:30 – 16:45 **Photoresponse Mechanism of Organic Field-Effect Transistors**
Dean Kos *et al.* *(Institute of Materials Science of Barcelona (ICMAB-CSIC))*

16:45 – 17:00 **Unraveling Atmosphere-Dependent Trap-Mediated X-Ray Detection in Organic Field-Effect Transistors**
Giulia Napolitano *et al.* *(University of Bologna)*

17:00 – 18:00 Poster Session

20:00 – 00:00 Social Party

Day 3

Wednesday, 16th September

Organic Functional Materials

Chair: TBA

09:00 – 09:30 **From Materials to Systems: Passive, Low-Energy Sensors Based on Organic Mixed Ionic–Electronic Conductors**
Tobias Cramer *(Invited Talk - University of Bologna)*

09:30 – 09:45 **Hydrophobic Film Formation at Electrified Interfaces and Its Impact on Hydrogen Evolution Reaction**
Nina Strasser *et al.* *(Ruhr-University Bochum)*

09:45 – 10:00 **Proton uptake mechanisms in benzimidazobenzophenanthroline (BBL)-based ladder-type materials**
Truyens Zoé *et al.* *(University of Mons, Belgium)*

10:00 – 10:15 **Conjugated polymer nanoparticles boosting growth and photosynthesis in biohybrid plants**
Manuela Ciocca *et al.* *(Free University of Bozen-Bolzano, Italy)*

10:15 – 10:30 **Agave Silk Fibers-Derived Nanocrystals Substrates for (Opto)electronic Bio-Interfaces**
Soufiane Krik *et al.* *(Free University of Bozen-Bolzano, Italy)*

10:30 – 11:00 **Coffee Break**

Bioelectronics and Memory Devices

Chair: TBA

11:00 – 11:30 **Molecular Recognition at the Gate: Aptamer-Functionalized OFETs for Biochemical Sensing**
Annalisa Bonfiglio *et al.* *(Invited Talk - Scuola Universitaria Superiore IUSS, Pavia, Italy)*

11:30 – 11:45 **Photoactive dendrites for neuromorphic and bioelectronic applications**
Matteo Boggiatto *et al.* *(Free University of Bozen-Bolzano, Italy)*

11:45 – 12:00 **Multimodal Organic Synaptic Phototransistors with Light-Emitting Functionality**
Stefano Toffanin *(Institute for Nanostructured Materials (ISMN), Bologna)*

12:00 – 12:15 **Multifunctional Organic PhotoTransistor: Integrating Volatile and Non-Volatile Memory in a Single Device**
Camilla Formento *et al.* *(Department of Chemistry G. Ciamician (UniBo), ISMN-CNR (Bologna))*

12:15 – 12:30 **Molecular Engineering of Side-Chains in Conjugated Polymers for Organic Memristors**
Jarmila Vilčáková *et al.* *(Centre of Polymer Systems, Tomas Bata University in Zlín, Czech Republic)*

12:30 – 14:00 **Lunch Break**

Organic & Hybrid Sensors and Devices 2

Chair: TBA

14:00 – 14:15 **Tailoring optoelectronic features and film organization through rational end-capping of thienopyrrole-fused benzothiadiazole semiconductors**
Matías J. Alonso-Navarro *et al.* *(Rey Juan Carlos University, Madrid, Spain.)*

14:15 – 14:30 **Epitaxy Meets Transfer Printing: A Pathway towards Organic Semiconductor Device Integration**
Alessandro Minotto *et al.* *(Università degli Studi di Milano-Bicocca)*

14:30 – 14:45 **Engineering Light with Defects: Vacancy-Driven Optical and Catalytic Functions in g-C_3N_4**
Alessandro Landi *et al.* *(Dipartimento di Chimica e Biologia Adolfo Zambelli, Università di Salerno, Italy)*

Awards and Closing Session

Chair: Organizing Committee

15:00 – 15:30 **Best Poster Award and Concluding Remarks**
(Organizing Committee)

Modelling materials with mixed ionic-electronic transport: from brute force to reduced models

Alessandro Troisi, Amali Guruge, Hesam Makki, Colm Burke, Kalyani Patrikar

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It is now possible to simulate the structure and dynamics with of mixed ionic and electronic conductors (OMIEC) by combining classical molecular dynamics and quantum chemical methods. The coupled dynamics of excess charges and nuclei is naturally included in the description and the methodology is scalable for the exploration of multiple chemistry. A key observation from these studies is an unexpected dynamical effect. The energy of the localized carrier states evolves in time with characteristic timescale of 5-500 ps, due to the conformational flexibility of the polymer and the interaction with the ions. The ionic and nuclear dynamics are driving the electronic dynamics rather than providing a static disordered landscape. As a consequence, large mobilities are possible also in the presence of very large disorders. A numerical model is derived to quantify the mobility enhancement due to the dynamic disorder and to link more transparently the physics of electronic transport in OMIEC with that of the most conventional "dry" semiconductors. The combination of brute force and reduced model is particularly powerful. Details models help exploring the details of the interactions between materials and biological environments while reduced models can be used to derive broader design rules. We show for example how there is an optimal bandwidth to maximize the charge mobility in organic semiconductors.

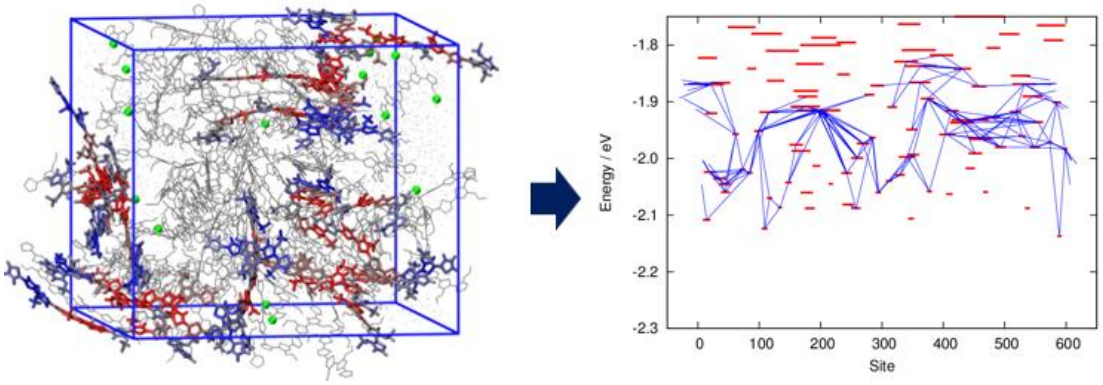

Figure 1. A model reduction scheme for OMIEC materials

[1] A G. Guruge, H Makki, A Troisi, *Macromolecules*, 2026, DOI: 10.1021/acs.macromol.5c02727
[2] R Herzhoff et al., *Mater. Horiz*., 2025, DOI: 10.1039/D5MH00610D
[3] C Burke, A Landi, A Troisi, *Mater. Horiz*., 2024, DOI: 10.1039/D4MH00706A
[4] Landi A. et al., *J. Mater. Chem. C*, 2023, DOI: 10.1039/D2TC05103F
[5] Keen S.T. et al, J. *Am. Chem. Soc*, 2022, DOI: 10.1021/jacs.2c02139

Ultra-Steep Switching and Trap-Minimized Interfacial Carrier Transport in Highly Layered Crystalline Organic Semiconductors

Tatsuo Hasegawa[1], Satoru Inoue[2], Kiyoshi Nikaido[1], Keito Murata[1], Shinji Tsuchida[1]

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We have demonstrated that a series of rodlike organic semiconductors (OSCs), composed of extended π-conjugated cores such as BTBT and BTNT linked with linear alkyl chains, exhibit exceptionally high layered crystallinity owing to the cooperative self-organization of their constituent molecular units [1−6]. These molecules form metastable layered liquid-crystalline phases at air–liquid interfaces, enabling the fabrication of large-area, highly homogeneous single-crystalline thin films through solution processing [7−10]. Depending on the π-cores and substituents, they also exhibit diverse layered structures, including polar molecular arrangements [11] and superlayer structures [12].

The pronounced layered crystallinity of these OSCs enables the formation of exceptionally clean semiconductor interfaces on highly liquid-repellent fluoropolymer insulating layers. As a result, organic field-effect transistors (OFETs) exhibiting near-ideal switching characteristics with subthreshold slopes approaching the theoretical limit have been realized [13−16]. In particular, the high interfacial quality significantly improves carrier injection and transport at the ternary interface composed of the electrode, semiconductor, and gate-insulating layers, enabling excellent transistor performance even in bottom-gate, bottom-contact (BGBC) devices.

Within these two-dimensional channel layers, interface trap states are substantially minimized, allowing transistor operation at carrier densities approximately two orders of magnitude lower than those of conventional inorganic FETs. This unique transport regime enables highly sensitive amplification of minute surface charges generated in soft piezoelectric materials, providing a promising platform for ultra-sensitive tactile sensing. In this presentation, we will discuss recent advances in layered OSC interfaces, ternary-interface transport physics, and related applications.

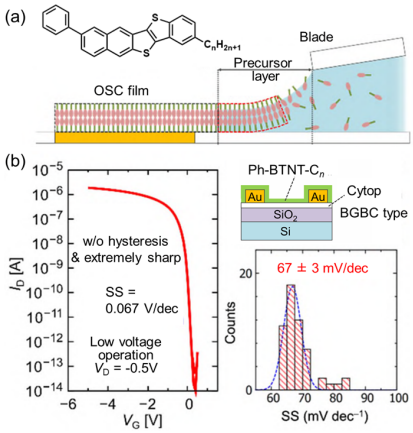

Fig. (a) Molecular structure of BTNT and solution processing. (b) Transfer characteristics of typical BTNT OFET.

References: [1] Hasegawa and Inoue, ***JSAP Review*** **2022**, 220206. [2] Inoue et al. ***Chem. Mater.*** **2018,** *30*, 5050. [3] Inoue et al. ***Chem. Mater.*** **2015**, *27*, 3809. [4] Minemawari et al. ***Chem. Mater.*** **2017**, *29*, 1245. [5] Inoue et al. ***Chem. Mater.*** **2022**, *34*, 72. [6] Higashino et al. ***Chem. Mater.*** **2024**, *36*, 848. [7] Yoneya et al. ***J. Phys. Chem. C*** **2017**, *121*, 8796. [8] Arai et al. ***Adv. Mater.*** **2018**, *30*, 1707256. [9] Nikaido et al. ***Adv. Mater. Int.*** **2022**, *9*, 2201789. [10] Nikaido et al. ***Phys. Rev. Mater.*** **2024**, *8*, 115601. [11] Inoue et al. ***Adv. Sci.*** **2024**, *11*, 2308270. [12] Nikaido et al. ***Sci. Adv.*** **2025**, *11*, eadv1878. [13] Kitahara et al. ***Sci. Adv.*** **2020**, *6*, eabc8847. [14] Murata et al. ***Phys. Rev. Appl.*** **2024**, *21*, 024005. [15] Murata et al. ***Phys. Rev. Appl.*** **2025**, *24*, 024038. [16] Tsuchida et al. ***Phys. Rev. Appl.*** **2025**, *24*, 024017.

Unraveling Exciton Transport and Self-Trapping in Conjugated Polymers

Llinersy Uranga-Piña 1, Royle Perez-Castillo 2, Beatriz Rodriguez-Hernandez 2, Maxim F. Gelin 3, Sergei Tretiak 4, Sebastian Fernandez-Alberti 2.

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Abstract Text: The study of excitons in π-conjugated polymers reveals a rich landscape of emergent phenomena critical to organic optoelectronics. These quasi-one-dimensional systems are defined by the strong interplay between electron-electron interactions, electron-nuclear coupling, and structural disorder, which collectively dictate their tunable optical, structural, and dynamical properties. Herein, we summarize recent theoretical advances, highlighting how these fundamental interactions govern exciton dynamics, particularly focusing on self-trapping and the complex nature of energy transport. We first present detailed atomistic simulations of the photo-induced response in artificial light-harvesting molecular antennas[1,2]. The computed transient absorption pump–probe (TA-PP) spectra monitor energy relaxation and redistribution in real time, and provide a detailed microscopic picture of the relevant energy-transfer pathways. We believe this represents the first reported on-the-fly atomistic simulation of TA-PP signals for such a large molecular system[2]. Further results offer atomistic insight into the conformational features associated with observed spectral trends, such as the red- and blue-shift in the absorption and fluorescence of three-dimensional cage-shaped molecules, respectively[3]. As a general trend, we find that internal conversion processes are mediated by a specific set of middle- to high-frequency normal modes, which directly influence the spatial exciton redistribution during the internal conversion, self-trapping, and intra-ring migration[4]. Our modeling shows that the nonadiabatic $S_2 \rightarrow S_1$ electronic transition activates specific collective asymmetric vibrational excitations of the polymer backbone. This activation promotes a periodic oscillatory evolution of the excitonic wave function before the excess energy dissipates into the thermal bath (i.e., the energy flow involves a transient, coherent motion governed by specific phonon modes)[5]. These studies demonstrate the potential of these molecular architectures for tunable exciton dynamics, enabling performance optimization for applications in light harvesting, energy conversion, and optoelectronics.

References:

[1] R. Perez-Castillo, et al., *Chemical Science*, **2025**, *16*, 13520.
[2] R. Perez-Castillo, et al., *Chemical Science*, **2024**, *15*, 13250.
[3] B. Rodriguez-Hernandez, , et al., *Journal of Physical Chemistry Letters*, **2021**, *12*, 224.
[4] B. Rodriguez-Hernandez, et al., *Physical Chemistry Chemical Physics*, **2020**, *22*, 15321.
[5] B. Rodriguez-Hernandez, et al., *Journal of Physical Chemistry C*, **2018**, *122*, 16639.

Phase behavior and electrical transport in DBTTF:HATCN donor–acceptor mixtures

Andreas Opitz[1], Hongwon Kim[2], Dmitry Lapkin[3], Gianfranco Melis[3], Ainur Abukaev[3], Marie Siegert[4], Lennart Frohloff[1], Lisa Schraut-May[4], Oleg Konovalov[5], Alexander Hinderhofer[3], Frank Schreiber[3], Jens Pflaum[4], Wolfgang Brütting[2]

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Abstract Text: The formation of donor–acceptor complexes (DACs) between the electron donor dibenzotetrathiafulvalene (DBTTF) and the acceptor hexaazatriphenylenehexacarbonitrile (HATCN) yields a phase with a distinct crystal structure and the emergence of sub-gap optical absorption bands absent in the pristine constituents. [1] Systematic variation of the mixing ratio, from pristine DBTTF to pristine HATCN, combined with X-ray scattering and atomic force microscopy, reveals pronounced composition-dependent changes in film structure and morphology.

Electrical measurements demonstrate a strongly non-monotonic dependence of conductivity on composition, with all mixed phases exhibiting substantially enhanced charge transport compared to the pristine films. Temperature-dependent studies of conductivity, charge carrier concentration, and mobility provide further insight into the underlying transport mechanisms. Notably, all mixed compositions display n-type behaviour, in contrast to pristine DBTTF. Ultraviolet photoelectron spectroscopy attributes this unexpected polarity to the electronic structure of the DAC, indicating that charge injection and transport are governed by the lowest unoccupied molecular orbitals of the DAC and HATCN.

Furthermore, the electrical performance is found to be critically modulated by morphology and structural ordering. These results establish a direct correlation between composition, electronic structure, and charge transport, providing a framework for the rational design of donor–acceptor systems with enhanced electronic functionality.

Reference: [1] A. Opitz et al., *Chemistry of Materials*, **2026**, published online, doi: 10.1021/acs.chemmater.6c00277.

Investigation of transport in OECTs with Electrochemical Strain Wave Microscopy

Filippo Bonafè[1], Junpeng Ji[2], Simone Fabiano[2], Beatrice Fraboni[1], Tobias Cramer[1]

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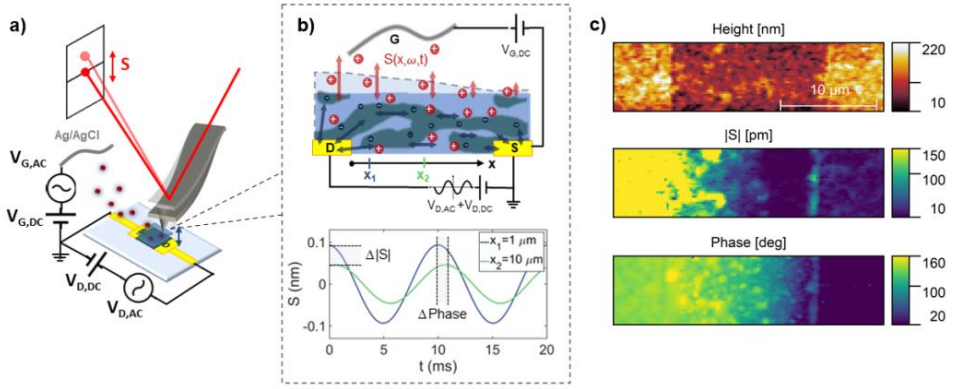
Critical advancements in organic electrochemical transistor (OECTs) for bioelectronic, neuromorphic, and sensing applications[1] require a deeper understanding of microscopic mixed ionic-electronic conduction processes governing device operation. In this work, we introduce electrochemical strain wave (ESW) microscopy to investigate transport processes in the OECT channel at microscopic length scales. ESWs are generated in mixed conductors by charge injection at the electrodes and propagate into the device channel through combined charge transport and swelling.[2] With AFM experiments we map the local amplitude and phase of ESWs in OECTs under different operating conditions. As a result, we demonstrate that quantitative ESW acquisitions can determine carrier concentration-dependent mobility effects in n-type and p-type devices, or reveal microstructural defects in the OECT channel altering local charge transport. Our findings provide a coherent framework to interpret the structure-functionality relation in OECTs, mapping transport properties below diffraction limit and without limitations by screening effects or electrochemical side reactions of the probe.[3]



Electrochemical strain wave microscopy on Organic Electrochemical Transistors (OECTs). a) Schematic of the experimental apparatus for mEC-AFM measurements of electrochemical strain waves (ESWs) propagating in OECT channels. b) Conceptual scheme correlating ionic and electronic transport with ESW propagation. c) mEC-AFM maps of local ESW amplitude and phase in operating BBL n-type OECTs.

References:

[1] A. Saleh, A. Koklu, *Nat Rev Bioeng*, **2024**, *2*, 559–574
[2] F. Bonafè, M. Bazzani, *Nat Commun,* **2025***, 16,* 2499
[3] F. Bonafè, J. Ji, *Small*, **2025**, *21*, 52

Understanding thermal transport in complex materials like organic semiconductors and metal-organic frameworks

Lukas Legenstein,[1,2] Florian Lindner,[1] Sandro Wieser,[1,3] Lukas Reicht,[1] Florian Unterkofler,[1] Marco Moser,[1] Simon Jamnik,[1] and **Egbert Zojer[1]**

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2: Chair of Physics, Montanuniversität Leoben, Leoben, Austria
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Abstract Text: Heat conduction is a crucial process for all applications in which excess heat needs to be either dissipated or supplied. In electrically insulating materials, heat transport can either be described in real space via the motion of atoms or in reciprocal space via the transport of phonons. To develop reliable structure-to-property relations for the thermal conductivity of complex materials, an atomistic understanding of the underlying processes is crucial. This understanding can be achieved via atomistic computer simulations provided that they yield quantitatively accurate results.

To achieve that, a highly accurate and at the same time extremely efficient description of inter-atomic interactions is required: as density functional theory (DFT) is far too inefficient for solving the Kohn-Sham equations millions of times for tens of thousands of atoms, and as classical force fields are far too inaccurate, system-specifically machine-learned force fields appear as the ideal choice. We applied so-called moment-tensor potentials trained via a specially adapted active learning approach,[1,2] reaching essentially DFT accuracy for various physical observables with a maximum estimated speedup of eleven orders of magnitude. These potentials can then be combined with methods operating in real space (analyzing particle trajectories)[1,3] and in reciprocal space (relying on phonon properties),[5-7] yielding a quantitative agreement with accurate experiments (often on single crystals).

As far as physical insights are concerned, for example, the analysis of the real-space effective temperature distribution in MOFs subject to a thermal gradient allows the identification of local heat-transfer bottlenecks;[3] in contrast, analyzing the dynamics of phonons reveals the actual heat-transport mechanism, showing that not only the particle-like motion of phonons, but also their tunneling becomes highly relevant.[4] Interestingly, it turns out that different ranges of phonons dominate different transport mechanisms.[6] Finally, changes in phonon properties explain why in molecular crystals like naphthalene the thermal conductivity increases by about an order of magnitude at elevated pressures of ~6 GPa.[7]

References: [1] Sandro Wieser and Egbert Zojer, *npj Comput. Mater.*, **2024**, 10, 18
[2] Lukas Reicht, Lukas Legenstein, Sandro Wieser, and Egbert Zojer, *Molecules*, **2024**, 29, 3724
[3] Sandro Wieser, Tomas Kamencek, Johannes P. Dürholt, Rochus Schmid, Natalia Bedoya-Martínez, Egbert Zojer, *Adv. Theory Simul.*, **2021**, 4, 2000211
[4] Lukas Legenstein, Lukas Reicht, Sandro Wieser, Michele Simoncelli, Egbert Zojer, *npj Comput. Mater.*, **2025**, 11, 29
[5] Lukas Reicht, Lukas Legenstein, Sandro Wieser, Egbert Zojer, *npj Comput. Mater.*, **2026**, 12, 129
[6] Florian P. Lindner, Marco Moser, Lukas Legenstein, Sandro Wieser, Egbert Zojer, submitted.
[7] Lukas Legenstein, Sandro Wieser, Michele Simoncelli, and Egbert Zojer, in preparation.

Universal free-energy scaling of quantum efficiency controlled by acceptor strength in organic solar cells.

Safakath Karuthedath[1,2*], Wenlan Liu[3], Neha Chaturvedi[1], Sri H. K. Paleti[1], Catherine S. P. De Castro[1], Abdul Azeez Hamsa[2], Jianhua Han,[1] Jafar I. Khan[1], Panagiota Kafourou[1], Joel Luke[1], Han Xu,[1] Yuliar Firdaus[1], Anirudh Sharma[1], Wejdan Althobaiti[1], Diego Rosas Villalva[1], Nicolas Ramos[4], Jaime Martin[4,5], Martin Heeney[1], Derya Baran[1], Thomas D. Anthopoulos[6], Denis Andrienko[3], Frédéric Laquai[1*], Julien Gorenflot[1*]

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Abstract

Y-family acceptors (A) have enabled organic solar cell efficiencies above 21%, yet the origin of their outstanding performance remains unresolved. To identify the governing factors, we compare

two Y-derivative acceptors, Y6 and ZY-4Cl, across binary blends with 11 different electron donors (D). We show that hole transfer (HT) at the D–A interface is the efficiency-limiting step, requiring an ionization energy offset of only ~0.3 eV for Y6 compared to ~0.6 eV for ZY-4Cl, set by interface energetics rather than π-stacking differences. Extending to an even wider range of systems, we find that external quantum efficiency universally scales with the Gibbs free energy for charge transfer, collapsing onto distinct trends defined by the strength of the acceptor's electron deficient end group. Stronger acceptor units yield a steeper efficiency rise, enabling high external quantum efficiencies at minimal energetic cost, largely independent of molecular family and challenging the perceived advantage of Y-derivatives.

Towards Circularly Polarised Luminescence from Inherently Chiral Inverted Singlet-Triplet Dyes

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Abstract Text: Recent years have seen rising interest in molecules that violate Hund's rule, where the first excited singlet state lies below the triplet (ΔEST< 0), accelerating reverse intersystem crossing, a key process in thermally activated delayed fluorescence. Such molecules hold potential for optoelectronic applications as OLEDs and photocatalysis.1,2 Despite growing interest, no single-molecule emission from a chiral dye with inverted gap has been reported, and only one case has shown such emission from supramolecular aggregates.3 We present a computational study on such inverted singlet-triplet (IST) molecules modified for chirality to enable Circularly Polarised Luminescence (CPL), an unexplored direction for IST emitters.

We show the first circularly polarised light emission (CPL) from a chiral molecule exhibiting inverted singlet-triplet gap. Our design is based on the achiral heptazine core,4 functionalised with chiral substituents. Photophysical characterisation, including temperature-dependent optical spectra and photoluminescence decay profiles confirms the inverted gap. Chiroptical properties show dissymmetry factor g~10-3 comparable to other chromophores functionalised with chiral groups. Combined with promising photoluminescence quantum yields, these findings highlight the potential of such materials for circularly polarised OLED devices.

We finally explored inherently chiral chromophores, focusing on extended triangulenes resembling helicenes,5 known for their strong CPL. Substituents enabling enantiomer separation were introduced, and racemisation barriers were evaluated. When inversion was lost, structures were further optimised, leading to a promising substrate combining a high barrier enabling enantiomer separation, strong CPL activity, and inverted singlet–triplet energetics, making it suitable for CP-OLED applications.

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Flipping the Rules:

From Inverted Singlet-Triplet Gaps to Diradical Switches

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Molecular platforms for optically addressable spin states are emerging as fascinating alternatives to solid-state spin centers, offering scalable synthesis, structural tunability, and chemical versatility.[1,2] In this talk, we present a molecular design strategy for achieving photoinduced spin polarization in organic diradicals bridged by systems featuring an inverted singlet-triplet (InveST) energy gap (see Figure 1).[3,4] These InveST units possess HOMO and LUMO orbitals localized on complementary atomic sites. By covalently linking the non-SOMO-bearing positions of alternant hydrocarbon radicals to the LUMO-localized atoms of the InveST bridge, we construct diradicals in which the radical centers remain electronically decoupled in the ground state, yielding degenerate singlet and triplet configurations. Upon photoexcitation, population of the InveST LUMO activates an excited-state exchange interaction between the radicals, generating a finite singlet-triplet gap and enabling spin-selective intersystem crossing to polarized triplet states. Using a combination of model Hamiltonians and multireference *ab initio* calculations, we establish design principles for tuning exchange interactions and spin-orbit coupling to achieve molecular-level control over optical-spin interfaces. The resulting InveST-bridged diradicals emerge as promising scaffolds for molecular quantum technologies.

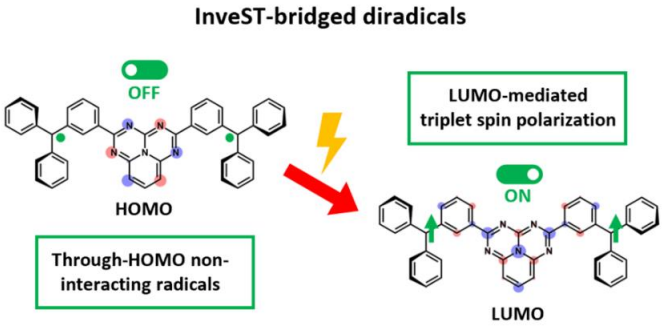

Figure 1 Schematic overview of the InveST-bridged diradical design and of the spin-spin locking as induced by the InveST-localized HOMO→LUMO transition.

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Tailoring Curcuminoid Synthesis for Surface-Patterned Optical Sensors and Sublimated Crystalline Electronic Frameworks

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Abstract Text: In recent years, curcuminoids (CCMois) have established themselves as molecular platforms[1] in various fields of nanoscience, extending beyond biological applications. These systems are linear and conjugated, and their straightforward synthesis allows for modifications to be made to different parts of their molecular structure. As a result, they offer a significant opportunity for the exploration of new materials with unique physicochemical features in the field of molecular electronics.[2-4] The effective combination of this chemical engineering with deposition methods enhances their suitability for different substrates, promoting surface organisation and the achievement of the enhancement of target properties. In this work, the FunNanSurf group applies a combination of these parameters and describes CCMoids covalently anchored to substrates for use as optical sensors,[5] as well as the development of soft-sublimation devices for the in-situ fabrication of electronic devices based on crystalline films of these materials,[6] alongside a discussión of their future propectives.

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Co-Crystallization and Charge-Transfer Complex formation in Thin Films: a strategy for NIR Sensing Applications

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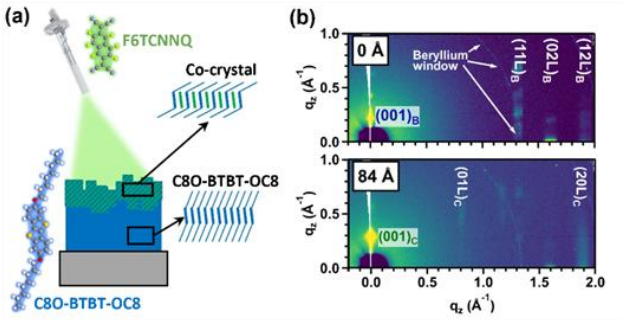
Charge-transfer complexes (CTCs) formed by the co-assembly of small conjugated molecules, typically an electron donor and acceptor, enable organic semiconductors with enhanced electrical and optical properties compared to their individual components, while avoiding complex synthetic routes [1–3]. Understanding and controlling co-crystallization in thin films is critical to exploit their properties in devices. Here, we investigate the formation of co-crystalline thin films comprising 2,7-bis(octyloxy)[1]benzothieno[3,2-b]benzothiophene (C8O-BTBT-OC8) and 1,3,4,5,7,8-hexafluoro-tetracyanonaphthoquinodimethane (F6TCNNQ) by sequential deposition of F6TCNNQ on C8O-BTBT-OC8 films, both vacuum sublimated. Grazing-Incidence Wide-Angle X-ray Scattering (GIWAXS) during acceptor deposition reveals the emergence and growth of the (001) Bragg peak associated with co-crystal formation. Atomic Force Microscopy (AFM) and Kelvin Probe Force Microscopy (KPFM) performed after acceptor growth confirms a morphological change in the films and an increase of the local work function. UV–vis spectroscopy demonstrates the formation of the CTC with a new absorption band in the near-infrared (NIR) absorption. We show that this approach is a viable strategy to grow uniform co-crystalline thin films, with potential application in NIR sensing applications.



(a) Schematic illustration of the sample preparation showing the deposition of F6TCNNQ (highlighted in green) onto a pre-formed C8O-BTBT-OC8 thin film (highlighted in blue) to form the co-crystal. **(b)** 2D GIWAXS maps acquired *in situ* before and after an 84 Å deposition of F6TCNNQ on C8O-BTBT-OC8, showing the emergence of co-crystallization.

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All-organic lasers with efficient near-infrared emission

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Abstract: Organic lasers are attractive light sources due to their advantages of chemical versatility, wavelength tunability, mechanical flexibility and low cost. Particularly successful for applications is the distributed feedback (DFB) laser, in which the device consists on a waveguide active film incorporating a diffractive grating. In this respect, the top-layer polymeric resonator architecture has demonstrated great success to obtain tunable devices with low threshold and high laser efficiency [1,2].

Our research group has intensively worked in this field, focusing in three main aspects: i) investigation of novel compounds towards the improvement of different laser parameters; (ii) development of methodologies to fabricate polymeric DFB resonators with different architectures; and iii) demonstration of the use of the prepared devices for sensing applications. In this presentation we will focus mainly in the first of these aspects, particularly on systems designed to obtain emission in the near infrared (NIR) spectral region, which is showing growing interest, driven by their potential applications in night vision devices, bioimaging and optical telecommunications. Thus, we will discuss results for various zig-zag nanographenes with extended conjugation either in 1D or 2D directions [3-5]; and a family of benzene-perylene ladder-type co-oligomers, all with very efficient and photostable laser performance [6].

On the technological side, we will also discuss our demonstration of a completely organic laser, including the active film, the resonator and the substrate [7]. This device has shown continuously tunable emission through bending, thus truly exploiting the mechanical flexibility advantage of organic materials, as well as successful operation for refractive index sensing.

The work has been funded by the MICIU/AEI/10.13039/501100011033 and by the ERDF/EU (grants PID2020-119124RB-I00 and PID2023-146660OB-I00) and by the Advanced Materials program through the Spanish MCIN, NextGenerationEU and by Generalitat Valenciana (grant MFA/2022/045)

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Tailoring optoelectronic features and film organization through rational end-capping of thienopyrrole-fused benzothiadiazole semiconductors

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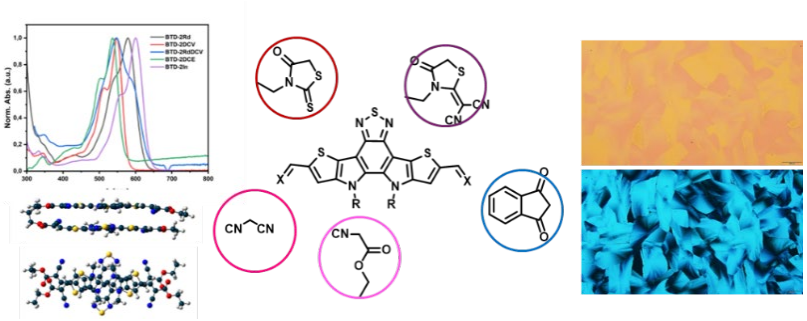
Abstract Text: Growing interest in sustainable energy technologies has strengthened the focus on π conjugated organic semiconductors, whose tunable structures offer promising electronic properties for next generation devices. Although Y6 type acceptors remain performance benchmarks in organic photovoltaics, their highly fused architectures require demanding and costly multistep syntheses,[1] motivating the exploration of simpler molecular frameworks capable of delivering competitive efficiencies through more accessible routes. In response to this challenge, and building on previous advances in the field,[2] we developed a new family of thienopyrrole fused benzothiadiazole (BTD) semiconductors bearing a range of strongly electron accepting end groups. This modular design enabled fine control over their optoelectronic properties, an approach supported by quantum chemical calculations that clarified the underlying structure–property relationships. To assess their potential for electronic applications, we investigated their thin film formation and charge transport behavior using bar assisted meniscus shearing (BAMS) to obtain controlled crystallization and reproducible morphologies.[3] Polarized optical microscopy and AFM provided insight into crystal orientation and domain structure under various deposition conditions, guiding the fabrication of organic field effect transistors (OFETs) used to evaluate charge mobility under optimized processing parameters.



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Multilayered perovskite heterostructures for photovoltaic applications

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Abstract Text: The presentation will review our recent collaborative work. Stable perovskite solar cells (PSCs) under operation were early demonstrated using 2D multilayered perovskite phases [1,2]. 3D perovskites are more promising in terms of high photoconversion efficiencies. Exploring the combination of 2D and 3D perovskites in PSC architectures is a joint project that started more recently. When combined in 2D/3D bilayer stacks using new versatile growth methods based on solvent engineering, excellent PSCs device stability can be achieved [3]. Besides solvent engineering, a deep understanding of electronic properties, including band alignment is required to properly choose each of the 2D and 3D layer compositions [4]. In addition, related work on 3D perovskite solar cells clearly demonstrated that strain management in the structure is key towards better stability under operation [5, 6]. Further improvements was achieved based on the concept of lattice matching [7], which relies on mechanical energy considerations to select the best pair of 2D/3D or more generally perovskite/perovskite combination. In 2024, it led to record stability for pure $FAPbI_3$ based PSCs [8]. Very recently, this stability was further improved by preventing the degradation pathway from 3C-$FAPbI_3$ to 2H-PbI_2 thanks to a Cl-based additive [9]. Instead, it undergoes degradation only upon exposure to harsh conditions such as 15-sun illumination and 90°C through the energetically 3R-PbI_2 phase path. These approaches are currently extended to combine more than a pair of perovskite layers of any type (3D, 2D, 1D, 0D…) and into solution-processed photoactive heterostructures to further improve stability, without compromising efficiency, in n-i-p or p-i-n PSC architectures, as well as for other optoelectronic devices.

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Flexible and High-Performance Perovskite-Polymer Composites for Dual X-Ray and Proton Direct Detection

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Abstract Text:

The growing demand for low-cost, lightweight, flexible, and scalable radiation detectors has stimulated interest in metal halide perovskites, which have rapidly demonstrated sensitivities exceeding those of conventional detector technologies. Here, we present flexible ionizing radiation detectors based on perovskite–polymer composites fabricated through a simple, low-cost, solvent-free mechanochemical process. Perovskite powders are synthesized by ball milling and embedded in a poly(butyl methacrylate) (PBMA) matrix, yielding composite materials that can be hot-pressed into free-standing pellets with thicknesses from 100 to nearly 500 μm. The resulting pellets are laminated onto substrates with patterned electrodes to fabricate hybrid photodetectors. The dry-processing approach enables reproducible, scalable manufacturing of thick active layers while avoiding solvents and complex deposition techniques. By optimizing the polymer content and processing conditions, stable devices with low dark current and reliable operation under ambient conditions are obtained. The composites exhibit excellent environmental stability and radiation hardness, making them suitable for long-term ionizing radiation detection [1]. To improve charge collection efficiency, both planar and vertical device architectures were investigated. Vertical geometry allows the electric field to be applied across the pellet thickness, leading to enhanced carrier extraction and doubling the sensitivity compared with planar devices. The polymer matrix also provides remarkable mechanical robustness. Devices laminated onto PET substrates maintain stable performance under repeated bending and achieve bending radii as low as 1 mm without significant changes in X-ray response, highlighting their potential for flexible radiation sensing applications [2]. Beyond X-ray detection, the devices were evaluated under a 5 MeV proton beam. Measurements demonstrate efficient proton detection, with thicker pellets benefiting from enhanced energy deposition and charge generation.

Finally, the influence of perovskite composition was explored by comparing all-inorganic and hybrid formulations. Hybrid perovskites containing methylammonium and formamidinium cations exhibited improved signal-to-noise ratios, likely due to enhanced defect tolerance and molecular dipole-assisted charge compensation. These results demonstrate that dry-processed perovskite–polymer composites provide a scalable route toward flexible, stable, and highly sensitive X-ray and proton detectors for next-generation radiation sensing and dosimetry.

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Hybrid 2D Perovskite Thin Films as a tunable platform for Fast and Thermal Neutron Direct Detection

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Abstract Text: The development of portable and flexible neutron detectors is essential for several applications ranging from nuclear safety and medical diagnostics to advanced radiation therapies and non-destructive testing. In contrast to charged particles and photons, neutron detection remains particularly challenging because neutrons poorly interact with matter through specific mechanisms depending on their energy. Consequently, the design of neutron-sensitive materials to be employed as active layers of efficient detectors requires careful tailoring of both composition and device architecture. Hybrid and organic semiconductors offer unique opportunities in this context. For fast neutrons, detection relies primarily on elastic scattering events that transfer energy to recoil nuclei. The presence of low-Z elements is therefore essential to maximize the energy transfer efficiency in the detection process. Organic and hybrid materials are intrinsically advantageous because they contain large fractions of light elements (i.e. H, C, N), providing a natural pathway for efficient fast-neutron conversion via elastic scattering. Here, we present a flexible thin-film detectors based on PEA_2PbBr_4 layered perovskite deposited from solution onto gold interdigitated electrodes on polyimide substrates. The devices provide stable real-time monitoring of fast neutrons in the 1–4 MeV energy range, generating electrical signals proportional to neutron flux. The micrometric thickness of the thin film active layer also reduces γ-ray interactions, contributing to improved neutron–gamma discrimination.
For thermal neutrons, efficient detection requires active materials containing specific isotopes with large thermal neutron-capture cross sections (e.g. ^{10}B, ^{6}Li). In this case, the versatility of organic and hybrid materials becomes particularly valuable, as their chemistry enables straightforward functionalization and integration of neutron-converting species within the active layer of the sensor by chemical molecular tailoring or by the incorporation of these species during the deposition from solution of these materials. We demonstrate this concept by incorporating ^{10}B-based conversion structures into the same detector platform employed for fast neutrons. Thermal neutron capture by ^{10}B generates energetic charged particles that are subsequently detected by the perovskite layer, enabling direct thermal-neutron detection.
These results highlight how hybrid perovskites can serve as a promising neutron-detection platform, where composition, functionalization and device design can be tailored to address different neutron sensing. More broadly, they illustrate the potential of solution-processable organic and hybrid materials for next-generation radiation detectors combining flexibility, scalability and radiation-specific tunability.

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All-Solution-Processed Perovskite Light-Emitting Transistors Enabled by Fully Organic Architecture

K. Zahoaliaj[1,2], A. Fappani[3], F. Pallini[3], V. Bellotti[3], N. Quaresima[1,2], M. Bolognesi[1], M. Prosa[1], L. Beverina[3], S. Toffanin[1]

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Abstract: $CsPbBr_3$ perovskite nanocrystals (Pe-NCs) are highly attractive solution-processable emitters for light-emitting applications because of their high brightness, narrow emission linewidth, and high photoluminescence quantum yield.[1] However, their integration into more advanced architectures such as organic light-emitting transistors (OLETs) is still limited by the scarcity of fully solution-processable platforms capable of supporting uniform and compact Pe-NC emissive layers (EMLs). Here, we report fully solution-processed perovskite-nanocrystal-based light-emitting transistors (Pe-LETs) employing $CsPbBr_3$ nanocrystals as the emitter. This is achieved through the development of a fully organic LET platform comprising a tailored bilayer gate dielectric based on polyvinyl alcohol and CyTOP®, a solvent-resistant p-type polymer semiconductor (DPP-DTT), and a nanocomposite EML formed by dispersing Pe-NCs in a PVK:OXD-7 matrix. Morphological and photophysical investigations, including confocal laser scanning microscopy, were used to optimize solvent choice and processing conditions for homogeneous film formation. The resulting Pe-LETs exhibit narrow electroluminescence at 509 nm with a full width at half maximum of 19.2 nm, demonstrating excellent color purity.[2] A maximum external quantum efficiency of 4.17×10^{-3} % was achieved, comparable to the best values reported for inorganic-based LETs.[3]

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Weak exciton–phonon coupling in two-dimensional perovskite thin films for high-performance UV photodetection

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Abstract Text: Two-dimensional layered perovskites have emerged as a compelling platform for flexible UV photodetection, combining tunable excitonic properties, high absorption coefficients, and compatibility with low-temperature solution processing on plastic substrates[1,2]. Here we investigate how film morphology, controlled through the choice of deposition method, shapes the excitonic landscape and ultimately determines the transport regime in flexible PEA_2PbBr_4 UV photodetectors.
We compare spin-coated and bar-coated films deposited on flexible polyimide substrates from identical precursor ink. Bar coating, which relies on directional meniscus-assisted spreading and slower solvent evaporation, produces films with markedly larger crystalline domains and reduced microstrain, as revealed by X-ray diffraction and optical microscopy. These structural differences are not merely morphological: temperature-dependent photoluminescence between 80 and 300 K shows that bar-coated films exhibit substantially weaker Fröhlich exciton–phonon coupling[3] for the delocalized excitonic transition and reduced inhomogeneous broadening, placing their optical response closer to that of a PEA_2PbBr_4 single crystal than any spin-coated counterpart.
The spectroscopic signatures translate directly into device behavior. Under 385 nm illumination, bar-coated photodetectors reach responsivities around 40 mA/W and specific detectivities above 10^{13} Jones at low optical flux, with dark currents below 100 fA, on par with state-of-the-art single-crystal perovskite detectors, but achieved here in a fully solution-processed, flexible architecture. Spin-coated devices remain in a trap-limited photoconductive regime, with responsivities two orders of magnitude lower, consistent with their stronger phonon coupling and higher structural disorder.
These results establish a direct, quantitative pathway from deposition method to excitonic landscape to transport regime, and demonstrate that bar coating can drive PEA_2PbBr_4 films from polycrystalline, disorder-dominated behavior toward quasi-single-crystal-like UV photodetection on flexible supports.

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Printable Electronics enabled by Supramolecular 2D Material Inks

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Two-dimensional (2D) materials have emerged as promising candidates for the Internet of Things (IoTs) and next-generation wearable electronics, owing to their exceptional properties and compatibility with solution- processed approaches, hence enabling the use of simple and cost-effective techniques – such as inkjet printing – for fabrication of flexible devices.

In this talk, I will present the development of biocompatible, water-based inks of conducting, semiconducting, and insulating 2D materials [1-2], based on the supramolecular chemistry approach that enables simultaneous exfoliation and functionalization of nanosheets, allowing to produce 2D materials with tailored surface chemistries, specifically designed for sensing and biomedical applications [3-4]. I will discuss fully printed photodetectors [2,5], memristors [6-7], and diodes [8] made onto paper. Finally, I will present the first flexible and fully solution processed 2D material transistor operating without ion-liquid gating. [9]

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Controlling Polymorphism in Organic Semiconductor Thin Films via Substrate Selection

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Organic molecular crystals are widely recognized as attractive materials owing to their well-known applicability in optoelectronic devices. Since polymorphism is frequently observed in these systems, fine-tuning the growth conditions represents an effective strategy to select the desired polymorph while providing insight into the intrinsic structure-property relationships of the material.

Within this context, dicyano-distyrylbenzene (DCS) compounds constitute a paradigmatic class of organic semiconductors that have attracted great interest because of the tunability of their emission color and efficiency, together with their intrinsic structural flexibility.[1]

Here, we focus on a β-DCS compound, namely (2Z,2'Z)-3,3'-(1,4-phenylene)bis(2-(3,5-bis(trifluoromethyl)-phenyl)acrylonitrile), hereafter referred to as CN-TFPA. Two monoclinic polymorphs exhibiting solid-state luminescence enhancement have been reported, characterized by luminescence in the blue (B-phase) and green (G-phase) visible regions, respectively.[2]

CN-TFPA films are grown via organic molecular beam epitaxy on an amorphous inorganic substrate, fused silica, and on an organic single crystal, namely (010)-oriented potassium acid phthalate (KAP). The morphology, structure, and orientation of the films are investigated by means of atomic force microscopy, X-ray diffraction (XRD), and polarized UV-visible and photoluminescence spectroscopy. The markedly different morphology and photophysical properties of the crystalline films reveal selective growth of the B-phase on silica and of the G-phase on KAP, demonstrating the key role of the substrate in inducing phase selection during growth, as also confirmed by XRD. More specifically, the selection of the G-phase on KAP is achieved through organic epitaxy, driven by the matching of surface corrugations via a line-on-line coincidence between the $[011]_{\text{G-PHASE}}$ and $<101>_{\text{KAP}}$ directions. Finally, an in-depth investigation of the optical properties of the films provides insight into the intrinsic optical response of the two polymorphs, enabling the assignment of the optical bands and their anisotropy.

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Operando Demonstration of Polymorphism–Performance Correlation in C8O-BTBT-OC8 OFETs

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Abstract Text:

Studying polymorphism in organic materials is of great importance because molecular packing in thin films can strongly influence carrier mobility in thin-film transistors (TFTs) and, consequently, device performance. [1]benzothieno[3,2-b]benzothiophene (BTBT) derivatives exhibit excellent charge mobility and air stability; however, the occurrence of polymorphism has limited the potential application of some BTBT derivatives in TFTs. For example, thin films of 2,7-bis(octyloxy) [1] benzothieno[3,2-b]benzothiophene (C8O-BTBT-OC8) exhibit a substrate-induced phase (SIP) when fabricated at room temperature, which differs from the bulk structure of single crystals. The SIP is metastable and has been reported to evolve into the most stable bulk phase over time.[1] Because the instability of structural phases can severely affect device performance, various post-processing methods, such as post-annealing and solvent vapor annealing,[2] are typically employed to achieve and maintain stable phases in devices.

We have previously reported[3] that thermal annealing of as-grown C8O-BTBT-OC8 thin films induces the formation of a high-temperature polymorph (HTP). However, the relationship between this thermally induced polymorphic transition and thin-film electrical performance remains insufficiently understood. In this study, we performed simultaneous operando GIWAXS and device characterization to investigate how the structural evolution of C8O-BTBT-OC8 thin films affects transistor performance during thermal treatment. This approach enables simultaneous tracking of thin-film polymorphic evolution and charge-transport behavior under device operating conditions, thereby directly establishing a correlation between structural changes and device performance. Our results demonstrate that controlling the stability of thin-film polymorphs is essential for improving the performance, operational stability, and reliability of organic electronic devices.

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Controlling Monolayer–Bilayer Transitions in Ph-BTBT-Cn Thin Films via Thermal Annealing and Molecular Mixing

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Abstract Text: Controlling polymorphism in solution-processed small-molecule semiconductors is essential for optimizing charge transport in organic field-effect transistors (OFETs). Here, we investigate the monolayer–bilayer phase transition in Ph-BTBT-Cn thin films via two complementary approaches: thermal annealing and molecular mixing. Structural characterization reveals that thermal annealing induces a well-defined transition from monolayer to bilayer polymorphs, resulting in enhanced vertical ordering and improved OFET performance.

Beyond thermal treatment, we explore molecular mixing in blends of Ph-BTBT-Cn and Ph-BTBT-Cn', where differences in alkyl-chain length molecular and molecular compatibility modulate self-assembly. Molecular mixing tunes intermolecular interactions, stabilizes intermediate polymorphic states, and enables access to bilayer-like layered structures that typically require thermal annealing in single-component systems. Electrical measurements confirm that these compositionally driven structural modifications lead to systematic improvements in OFET characteristics.

Overall, this work establishes molecular mixing as a viable and complementary strategy to thermal annealing for engineering polymorphism and enhancing charge transport in organic semiconductor thin films.

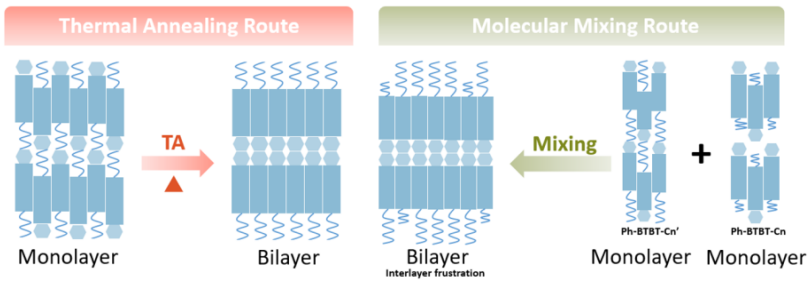

Figure 1. Thermal annealing and Molecular mixing routes to Monolayer-Bilayer transition

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Alkyl Chain Length Controls Polar Phases Stability in Asymmetric BTBT Thin Films

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Understanding the structure and polymorphism of organic electronic materials is essential for optimizing device performance. A representative example is 7-decyl-2-phenyl[1]benzothieno[3,2-b][1]-benzothiophene (Ph-BTBT-C_{10}), where high charge carrier mobility is related to a structural transformation from a metastable thin-film phase to a stable bilayer phase with a head-to-head configuration [1]. Such configuration cancels the intrinsic longitudinal electric dipole moment that results from the asymmetric molecular structure. In our previous work, Kelvin Probe Force Microscopy (KPFM) revealed a polar polymorph in Ph-BTBT-C_{10} thin films, arising from unidirectional molecular stacking [2].

Here, we extend this study to a series of asymmetric BTBT derivatives with a varying alkyl chain lengths (n = 4, 8, 12) by combining KPFM and Grazing Incidence Wide Angle X-ray Scattering (GIWAXS). This study examines systematically the effect of alkyl chain length on the formation and thermal stability of polar phases. Short-chain derivatives (n = 4) exhibit a thermally stable polar polymorph (Fig.1b), whereas longer chains ($n \geq 8$) favour a transition toward non-polar bilayer structure, as evidenced by a decrease in surface potential relative to the substrate with the temperature (Fig.1c). The findings establish polar polymorphism as a general feature of asymmetric BTBT derivatives and demonstrate that its stability can be tuned through molecular design. This enables control of built-in dipolar electric field in thin films, offering a route to control the optoelectronic properties of organic semiconductors.

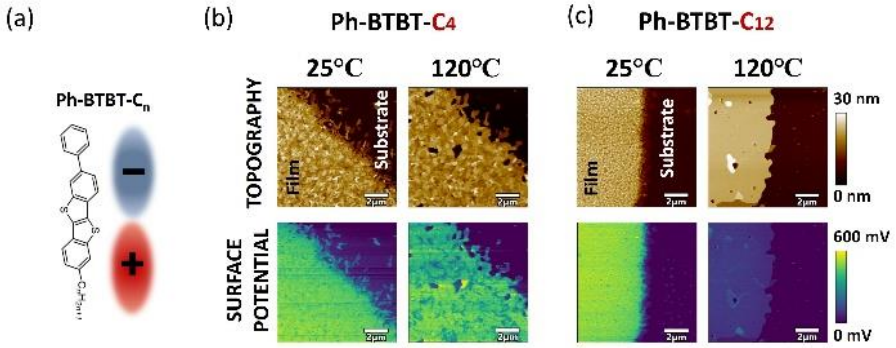

Figure 1. (a) Chemical structure of Ph-BTBT-Cn derivatives with scheme of the electrostatic distribution. KPFM measurements during *in situ* annealing of (b) Ph-BTBT-C12 film and (c) Ph-BTBT-C4 film, showing the evolution of the topography (top panels) and the surface potential maps (bottom panels) with the temperature.

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Galvanic Molecular Intercalation for Hybrid 2D Electronics

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Abstract Text: Molecular functionalization has become a central strategy in organic and hybrid electronics, enabling the tuning of charge injection and dielectric environment through the chemical versatility of molecular systems. In recent years, these concepts have also been extended to 2D materials, where molecular species have been employed to tailor electronic and optoelectronic behavior. However, since these strategies rely on surface modification, their impact is often limited to exposed surfaces and ultrathin flakes.

Molecular intercalation offers an attractive alternative by inserting functional species directly within the van der Waals gaps of layered materials, creating buried organic/inorganic interfaces throughout the crystal volume. This approach enables the formation of hybrid superlattices in which molecular functionalities can directly tailor the intrinsic physical properties of bulk crystals. Despite this potential, molecular intercalation in 2D materials remains comparatively underdeveloped, largely because conventional methods often degrade crystalline quality and are difficult to apply to nanodevices.

Here we introduce a galvanic intercalation strategy that exploits the low reduction potentials of selected metals to drive the insertion of molecular cations under mild conditions.[1] The method enables the incorporation of a broad range of functional species—including organometallic complexes and chiral molecules—into both bulk crystals and few-layer flakes of vdW materials. Using this platform, we investigate how molecular intercalation modifies the electronic transport of the van der Waals superconductors $NbSe_2$ and TaS_2 within the same few-layer devices before and after intercalation.[2]

In parallel, the galvanic approach enables the fabrication of more complex hybrid architectures, including vertical intercalation heterostructures in which molecules are selectively confined to one component of a van der Waals stack, and lateral heterostructures where different molecular species occupy neighbouring regions of the same flake. Finally, we show that these intercalated materials can be integrated into superconducting devices,[1] highlighting galvanic molecular intercalation as a versatile platform to engineer hybrid functionalities and emergent electronic states in 2D materials.

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Self-assembled pentacene on monolayer WS_2: a bottom-up route to a type-II organic/TMD heterostructure

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Abstract **Text:**

Hybrid van der Waals heterostructures combining transition metal dichalcogenides (TMDs) and organic semiconductors are promising platforms for tuning interfacial electronic properties[1] and for orbital-resolved studies of charge transfer and energy-level renormalization[2], [3]. Here, we investigate the pentacene/monolayer WS_2 interface by combining scanning tunneling spectroscopy (STS), photoemission orbital tomography (POT) and G_0W_0 calculations. In particular, pentacene self-assembles into an ordered monolayer on WS_2, forming a heterostructure with type-II band alignment. A key requirement for obtaining a structurally ordered interface with a well-defined electronic structure is an extended, atomically flat monolayer WS_2, most reliably achieved by bottom-up growth. We therefore employ fast epitaxial growth of WS_2 on Au(111) using DMDS as a safer sulfur precursor, while Au(111) provides an atomically clean template and the conductivity needed for STS and POT measurements. STS probes occupied and unoccupied states locally, but in monolayer WS_2 the fundamental gap cannot be reliably extracted from tunneling spectra alone because states with $k \neq 0$ are strongly attenuated. POT resolves this ambiguity by identifying pentacene- and WS_2- occupied states in momentum space and, together with G_0W_0, enables a reliable determination of pentacene HOMO position with respect to WS_2 valance band maximum (VBM), demonstrating the establishment of a type-II band alignment.

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Graphene-Metal interfaces: correlating structural and electrical characterization with defects and doping in Raman as a function of contact resistance.

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The contact resistance of graphene/metal interfaces is a crucial parameter that affects the performance of devices based on graphene. A high contact resistance can limit the current in graphene-based field effect transistors (GFET),[1] and is currently the main factor limiting the radio-frequency bandwidth in graphene phase modulator.[2] The integration and down-scaling of graphene electronic devices present an important challenge in the development of a Complementary Metal-Oxide-Semiconductor (CMOS) compatible process, that enables the reproducible formation of low contact resistance.[3] However, the origin of contact resistance has still space for debate, since no direct spectroscopic characterization can be performed on working devices. We present a robust approach to investigate the graphene-metal interface in top metallic contacts of operational devices using Raman spectroscopy. A transparent substrate, suitable for visualization and processing of graphene, was optimized by tuning the thickness of Aluminium and amorphous Silicon Nitride on top of a glass substrate. After photolithography and deposition of Cr/Au contacts, the graphene-metal interface was exposed to Raman investigation, using the 457 nm laser excitation. Additionally, electrical characterization was performed on the same devices: sheet resistance was obtained using Van der Pauw configuration and contact resistance was determined using the transfer length method. The technique proposed here permits to correlate the obtained increase in the D signal and decrease in the 2D signal at the graphene-metal interface, with the electrical parameters of graphene-metal contact.[4]

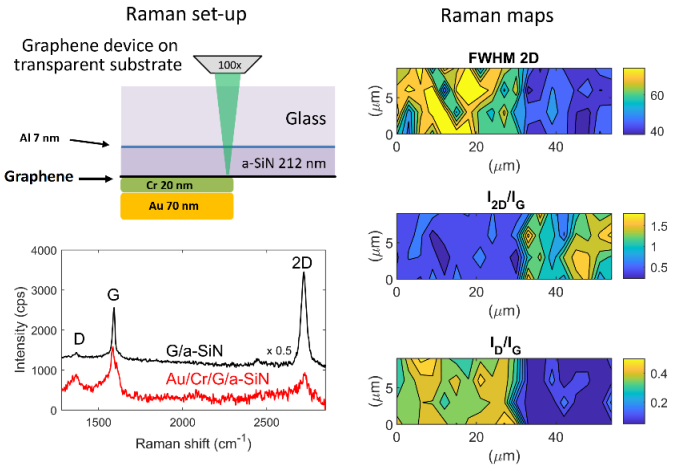

Figure. Proposed Raman set-up for investigation of graphene/metal interface in operative devices [4]

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Critical role of polymer gate dielectrics on the charge carrier transport in perovskite field-effect transistors

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Understanding the role of interfaces in organic and hybrid devices remains critical for advancing their optoelectronic applications. Despite these impressive advances in organic [1] and hybrid semiconductors [2] the role of the semiconductor/dielectric interface, where in the transistor the charge transport predominantly occurs, has remained poorly understood. Most studies focus on bulk film properties, leaving a critical gap in understanding of how interfacial chemistry governs charge carrier transport and thus device performance.

In this work [3], we address this aspect challenge by systematically investigating polymer gate dielectrics with different dielectric constants as interlayers on inorganic SiO_2 in perovskite field-effect transistors, more specifically we used phenethylammonium tin iodide ($(PEA)_2SnI_4$) as a model semiconductor. Our results reveal that high-k polymer dielectrics induce strong dipolar disorder at the interface, which localizes charge carriers and lowers in this way their transport resulting in unreliable device behavior. In contrast, low-k polymers reduce the interfacial charge localization and effectively passivate hydroxyl trapping groups on SiO_2, leading to stable perovskite transistor operation. These findings not only elucidate the chemical origins of interfacial charge trapping and localization but also provide clear guidelines for designing dielectric interfaces to optimize both electronic performance and operational stability of perovskite transistors. The comprehensive insights on the role of polymer dielectrics on the charge transport are relevant also for other types of semiconductors and therefore important for a broad scientific community.

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Electrolyte-gated organic field-effect transistors for point-of-care sensing

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Electrolyte-gated organic field-effect transistors (EGOFETs) are emerging as powerful, ultrasensitive, label-free biosensors due to their low cost, straightforward electrical readout, and inherent signal amplification. Their operation is based on the formation of two electrical double layers (EDLs) at the organic semiconductor–electrolyte and electrolyte–gate interfaces when a gate voltage is applied. This interaction modulates charge transport along the organic semiconductor, rendering EGOFETs highly responsive to interfacial changes—a property extensively harnessed in biosensor development.

A common approach for biosensor fabrication involves the biofunctionalization of the gate electrode using antibody or aptamer immobilization strategies. Such methodologies have enabled the detection of biologically relevant molecules at ultra-low concentrations, positioning EGOFETs as promising candidates for next-generation point-of-care (PoC) diagnostics. For instance, in our group, we have leveraged this platform to detect alpha-synuclein, a biomarker of Parkinson's disease and to monitor the aggregation kinetics of beta-amyloids [1–2].

Despite their diagnostic potential, the portability of EGOFET-based assays is often hindered by limited microfluidic integration and labor-intensive, multi-step protocols. To overcome these limitations, we present a simplified EGOFET integrated with lateral flow paper fluidics, enabling a reusable, compact, and cost-effective PoC test with rapid turnaround (~30 minutes). This platform was validated for the detection of Human Immunoglobulin G and to detect Hepatitis B/C biomarkers, demonstrating a broad linear range, high selectivity, reproducibility, and very low limit of detection [3-4].

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Photoresponse Mechanism of Organic Field-Effect Transistors

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Abstract Text:

This work uncovers the fundamental mechanism of optical photoresponse in organic phototransistors. Through a rigorous study of the electrical and optical factors that generate photoresponse, we find that photoresponse originates from trapping of charge carriers at the semiconductor-dielectric interface, producing a photo-induced gating effect. Crucially, trapped charges originate from exciton dissociation driven by the electric field near the drain and source electrodes. A minimum electric field of ~0.5 V/nm is required to trigger dissociation and trapping, and thus produce photoresponse.

We obtain these results by scanning a tightly focussed laser across the transistor channel while simultaneously acquiring transistor transfer characteristics, observing highly localized shifts in the turn-on voltage in real time. These shifts correlate systematically with illumination dose, location, and source-drain-gate voltages, while leaving the carrier mobility largely unaffected. We find that charges originating from exciton dissociation have a diffusion radius of 5 µm, and they can be trapped very deeply and at high concentrations leading to remarkable turn-on voltage shifts in excess of 60 V. Kelvin probe force microscopy confirms the formation of negatively charged regions along the illumination path, consistent with exciton dissociation followed by electron trapping at the semiconductor-dielectric interface. Numerical simulations illustrate the potential landscape inside the channel, supporting the model of exciton dissociation near the electrode boundaries. The mechanism is robust across multiple high-performance organic semiconductors, including TMTES-pentacene, TIPS-pentacene, and diF-TES-ADT, and is independent of grain boundaries or crystal morphology.

Our fundamental discoveries represent a step change in our understanding of photoresponse in organic devices, and will drive rational development of highly sensitive photodetectors and optoelectronic memories.

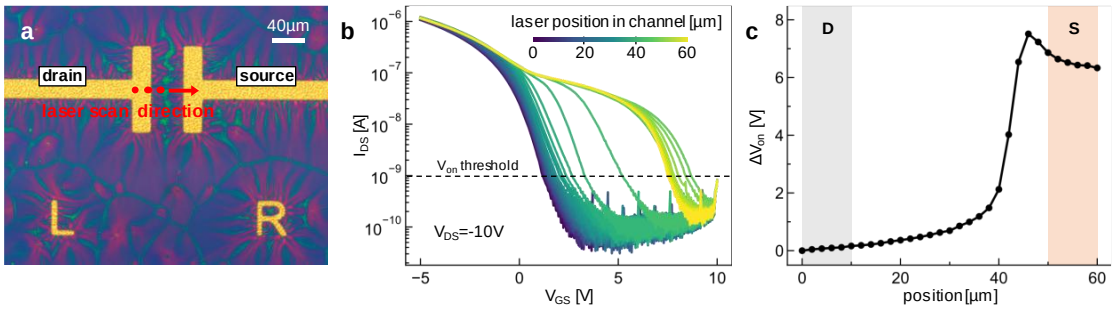

Figure 1. **a**, Geometry of the phototransistor: the channel between drain and source is scanned by a focussed laser beam. **b**, Transistor transfer characteristics are acquired in real time as the beam is scanned across the channel, producing a sharp shift in turn-on voltage. **c**, The shift in V_{on} voltage is concentrated at the source electrode interface.

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Unraveling Atmosphere-Dependent Trap-Mediated X-Ray Detection in Organic Field-Effect Transistors

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Abstract Text: Organic field-effect transistors (OFETs) represent a promising class of devices for ionizing radiation detection and dosimetry, owing to their mechanical flexibility, compatibility with large-area, low-cost fabrication, and tissue-equivalent composition. [1] However, their operation as detectors is often limited by environmental instability, since oxygen and moisture can strongly affect charge transport and promote the formation of radiation-induced trap states. [2] Encapsulation is therefore a promising route to improve device stability and control the detector response by limiting the interaction between the organic semiconductor and the surrounding atmosphere. [3] Here, we study the role of Parylene-C encapsulation in determining the electrical stability and X-ray response of OFET-based radiation detectors. By comparing coated and uncoated devices under controlled atmospheric conditions, we show that non-encapsulated OFETs display a strongly environment-dependent response. In air, interactions with oxygen and water modify both the sensitivity and transient dynamics through the formation of trap states. Under vacuum, the response is instead governed by long-lived charge trapping, leading to a more pronounced cumulative dose dependence. Parylene-C encapsulation produces a similar stabilization effect, leading to an integrative response that is no longer dependent on the external environment. Under 150 kVp X-ray irradiation, encapsulated OFETs achieve a maximum threshold-voltage sensitivity of (109 ± 2) mV/Gy, comparable to values reported for state-of-the-art CMOS-based RADFET dosimeters. These results show that Parylene-C encapsulation does not merely improve device stability but also plays an active role in defining the radiation detection mechanism. This work highlights encapsulated organic transistors as promising candidates for flexible, tissue-equivalent, and integrative dosimetry platforms.

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From Materials to Systems: Passive, Low-Energy Sensors Based on Organic Mixed Ionic–Electronic Conductors

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Abstract:

Organic mixed ionic–electronic conductors (OMIECs) are promising materials for bioelectronics and electrochemical sensing due to their ability to couple ionic and electronic charge transport at low operating voltages. Realizing fully passive and battery-free sensor systems based on OMIECs, however, requires understanding the fundamental limits of signal propagation and energy dissipation in these materials.

Here, we first investigate dissipative charge transport in OMIEC channels using electrical phase velocity measurements and modulated electrochemical atomic force microscopy.[1] Interpreting the results within a transmission line framework reveals that energy dissipation is governed by the ratio between electronic mobility and volumetric capacitance, establishing a key figure of merit for OMIEC materials beyond transistor amplification.

Building on this understanding, we demonstrate a fully passive oxygen sensor based on an organic electrochemical transistor (OECT).[2] By combining optimized device geometries with near-field communication (NFC) power harvesting, the system enables wireless and battery-free oxygen sensing in air and water. The interrogating NFC field is sufficient to power the electronics, acquire the sensor signal, and transmit the data wirelessly.

These results connect microscopic transport physics with the development of sustainable, ultra-low-power sensing systems based on OMIEC materials.

Keywords:

Organic mixed ionic–electronic conductors, Organic electrochemical transistors, Passive wireless sensing, Low-power bioelectronics, Near-field communication sensors

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Hydrophobic Film Formation at Electrified Interfaces and Its Impact on Hydrogen Evolution Reaction

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Abstract Text: Understanding the molecular structure of aqueous interfaces at electrified metal surfaces is central to electrochemical reactivity, in particular for processes such as the hydrogen evolution reaction (HER). Classical continuum descriptions fail to capture key molecular features such as hydrogen bonding and density fluctuations, which critically govern interfacial chemistry.

Molecular dynamics simulations at constant applied potential for the gold-water interface, a model system for electrocatalytic surfaces, reveal pronounced interfacial structuring. [1] While the first water layer forms a highly ordered, two-dimensional hydrogen-bond network, the adjacent layer shows strongly reduced connectivity. This results in a local depletion of water density and the formation of interfacial cavities, indicative of hydrophobic structuring that can alter reactant accessibility and solvation.

To experimentally probe these effects, we employ terahertz (THz) spectroscopy under externally controlled electric fields, providing access to collective intermolecular vibrations and thus the hydrogen-bond network at charged interfaces. [2] This approach enables the direct observation of hydrophobic, cation-rich interfacial films that significantly restructure the electric double layer. [3] By systematically varying tetraalkylammonium-based cations and electrolyte composition, we demonstrate how ion-specific interactions control the formation and stability of such interfacial films.

Combining THz spectroscopy with molecular dynamics simulations allows us to rationalize the underlying molecular mechanisms. These findings highlight that hydrophobic interfacial films can strongly influence water structure, proton availability, and interfacial transport processes, thereby modulating HER activity. Depending on their composition and stability, such films may either enhance or inhibit the HER, providing a potential handle to tune electrocatalytic performance.

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Proton uptake mechanisms in benzimidazobenzophenanthroline (BBL)-based ladder-type materials

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Electrochemical proton storage is key to the development of next-generation high-rate energy storage devices such as aqueous batteries. To improve their performance, it is fundamental to manage how electrochemically doped materials interact with ions. Achieving this demands a molecular-level insight into how ion uptake, solvation, and structural organization change throughout electrochemical doping [1, 2].

In this work, we first focus on a side-chain-free electron-transporting organic mixed ionic–electronic conductors (OMIEC) exhibiting highly reversible doping behavior, namely poly(benzimidazobenzophenanthroline) (BBL) (Figure 1a). We model and quantify the interactions between its monomeric unit and various counterions, across different electrochemical doping levels. In collaboration with experimental partners, we identify the preferred interaction sites and elucidate the mechanisms governing proton uptake. These mechanistic insights provide a framework to rationalize experimentally observed behaviors, such as water expulsion and deswelling of BBL films under applied bias [1].

We then extend this approach to a two-dimensional system based on the same redox-active unit, combined with triphenylene cores to form a ladder-type covalent organic framework (2D COF), denoted 2D BBLTP (Figure 1b) [2]. Incorporating redox-active units into porous 2D frameworks represents a promising strategy to overcome the intrinsic capacity and energy density limitations of organic materials [3]. Using first-principles calculations and tight-binding models, we investigate the impact of proton uptake on the magnetic and electronic properties of the COF monolayer.

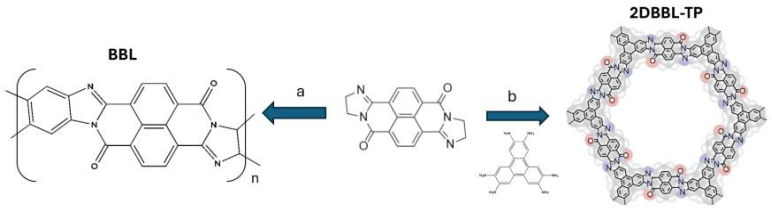

Figure 1: Redox-active unit of interest as the building block of a) poly(benzimidazobenzophenanthroline) and b) ladder-type 2DBBL-TP

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Conjugated polymer nanoparticles boosting growth and photosynthesis in biohybrid plants

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Abstract Text: Engineered nanomaterials integrated into photosynthetic systems could pave the way to new, exciting avenues towards biohybrid systems and renewable energy sources [1,2]. Here, a biohybrid plant developed through the integration of poly(3-hexylthiophene) nanoparticles (P3HT-NPs, Ø ca. 100 nm [3]) in *Arabidopsis thaliana* plants is presented (Fig.1) [4]. P3HT-NPs were used to enhance plant solar radiation absorption, with a spectrophotometric profile matching chlorophyll absorbance. The P3HT-NP-engineered biohybrid plants showed a 45% increase in root length, corresponding to a relevant enhancement in biomass production of up to 17% compared to the control group. The presented biohybrid plant might open a new route for improving CO_2 capture and oxygen production, underscoring the transformative potential of combining nanomaterials with plant biology, and paving the way for novel biohybrid nano-engineered renewable energy sources.

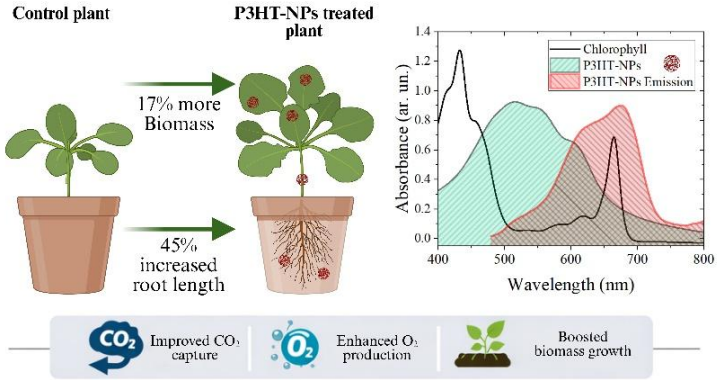

Figure 1: Biohybrid plant schematics and absorption spectra of P3HT-NPs and chlorophyll, highlighting enhanced light-harvesting capability. Created in https://BioRender.com

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Agave Silk Fibers-Derived Nanocrystals Substrates for (Opto)electronic Bio-Interfaces

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Abstract Text: Understanding and engineering interfaces in organic and hybrid electronic systems is critical for advancing (opto)electronic technologies spanning energy conversion [1], sensing [2], and biointerfaces [3]. However, the development of sustainable, optically transparent, mechanically stable and biologically compatible devices, represents a key challenge [4]. As the substrate generally accounts for the largest fraction of a flexible optoelectronic device in terms of both mass and volume, the selection of its materials is of critical importance from a sustainability standpoint. Here, we introduce a biodegradable and flexible substrate based on Agave Silk Fibers-derived nanocrystals (ASF-NCs), designed to enable optical and electronic coupling at organic and bio-hybrid interfaces (Figure 1).
The fabricated ASF-NCs substrate (avg. thickness 17.8 ± 1.5 µm) exhibits good optical transparency in the visible-near-infrared (NIR) spectral range (300-900 nm) combined with mechanical flexibility providing favourable interfacial conditions for organic semiconductors (OS) and photoactive materials. Its nanostructured morphology supports deposited OS layers (e.g. poly(3-hexylthiophene-2,5-diyl) (P3HT), chlorophyll) enabling efficient light–matter interaction while maintaining conformability for soft and irregular surfaces.
Biodegradability assessments demonstrate rapid degradation in aqueous environments confirming the potential of this substrate for transient biomedical applications.
The combination of optical transparency, flexibility, and bio-derived composition positions the ASF-NCs substrate as a versatile platform for phototransistors, photodetectors, and (opto)electronic devices in general. This work opens new avenues toward sustainable and biologically integrated (opto)electronic systems.

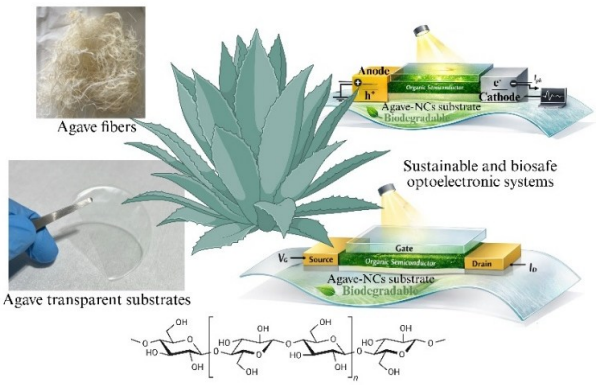

Figure 1: Conceptual schematics of sustainable and biosafe optoelectrical systems based on Agave-NCs substrates. Created in https://BioRender.com

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Molecular Recognition at the Gate: Aptamer-Functionalized OFETs for Biochemical Sensing

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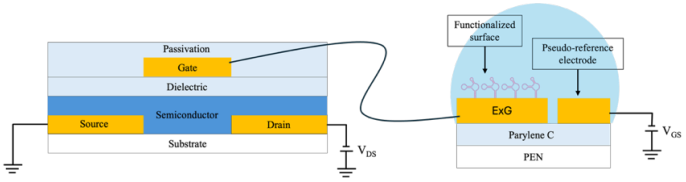
Organic Field-Effect Transistors (OFETs) have emerged as versatile transduction platforms for biochemical sensing, owing to their mechanical flexibility, low-cost fabrication, and compatibility with large-area processing. A particularly attractive configuration couples the transistor with a physically separated sensing surface acting as an extended gate (ExG): this solution has recently showed very interesting performances for ion sensing [1]. Beside the intrinsic signal amplification, the main advantage of ExG-OFETs is the possibility of selectively functionalizing the ExG area without directly exposing the organic semiconductor to the biological environment, thus improving shelf life and operational stability. In this work, we present an ExG-OFET platform in which the interface properties of the sensing electrode are engineered to achieve selective biochemical detection. The sensing unit consists of a gold extended-gate electrode functionalized with thiolated DNA aptamers via a controlled self-assembly protocol. Target binding at the gold/aptamer/electrolyte interface induces a conformational change in the aptamer structure and charge distribution, modulating the surface potential and producing a measurable shift in the OFET drain current. This transduction mechanism places interface engineering at the core of device performance, making the platform directly relevant to the study of interface properties in organic electronics.



As a demonstrative application, the platform was employed for cortisol detection in buffer solution, a relevant stress biomarker present in biofluids such as sweat [2]. A systematic comparison between a short (14-mer) and a long (61-mer) thiolated aptamer sequence revealed that aptamer length is a critical design parameter: in particular, the long aptamer yielded a clear, reproducible, concentration-dependent current modulation across a pM–µM range. These results point to aptamer length as a key factor governing charge coupling efficiency at the bioelectronic interface. Stability measurements performed in pure buffer confirmed negligible drift, validating the robustness of the functionalization protocol. Complementary surface characterization via Surface Plasmon Resonance (SPR) is currently underway to provide independent validation of aptamer binding and surface coverage, further corroborating the interface-level interpretation of the electrical response.

The modularity of the ExG-OFET architecture — where the sensing surface can in principle be functionalized with bioreceptors targeting diverse analytes — positions this platform as a general-purpose tool for label-free biochemical detection. Potential applications include wearable and point-of-care devices for continuous monitoring of biomarkers in sweat and other biofluids.

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Photoactive dendrites for neuromorphic and bioelectronic applications

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Abstract Text: Organic mixed ionic-electronic conductors (OMIECs) have played an essential role in helping to emulate the dual ionic and electronic pathways of biological signaling [1]. In OMIECs, ion penetration from the electrolyte alters the material's properties with temporal dynamics that can depend on prior stimulation history, opening the way to studies of synthetic analogs of synaptic plasticity. Organic dendritic networks based on poly(3,4-ethylenedioxythiophene) (PEDOT) have already demonstrated an effective route to biologically inspired computing, giving rise to complex dynamics that resemble the way the brain computes [2].

A persistent limitation of these platforms is their reliance on global electrical inputs, which precludes spatially selective addressing within a single network. Optical stimulation offers a natural route to this missing spatial degree of freedom. Poly(3-hexylthiophene) (P3HT) is an attractive candidate for this, being a biocompatible phototransducer widely used in biological interfaces [3].

Here we present a route to obtain optically active P3HT dendritic fibers through electropolymerization. We demonstrate that the resulting distributed polymer/electrolyte interface is capable of accumulating ions upon illumination, shifting the open circuit potential of the electrolyte by tens of millivolts within seconds. This shift persists in time, giving rise to short-term memory effects, together with paired-pulse facilitation (PPF) with a characteristic time of 14.2 s, thereby opening the possibility of neuromorphic applications. Finally, we show how the resulting fibers can be embedded in the biological environment, enabling light-driven stimulation of living cells. These results open the way to a spatially resolved, multimodal neuromorphic interfaces.

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Multimodal Organic Synaptic Phototransistors with Light-Emitting Functionality

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Abstract: Neuromorphic computing, inspired by the operating principles of the human brain, uses physical artificial neurons for computation and has attracted growing interest in recent years.[1] In parallel, optical neural networks are emerging as an efficient information-processing approach due to their high speed, parallelism, and low energy consumption.[2] Combining these two concepts in hybrid optoelectronic systems is particularly appealing, as it merges the adaptive and memory-like behavior of synaptic devices with the fast signal processing capabilities of light. Here, we present a multimodal organic synaptic phototransistor with light-emitting functionality based on a hybrid dielectric architecture incorporating a persistent radical (PyPBTM)[3]-doped polymethylmethacrylate dielectric layer. This design enables light sensing, light emission, short-term electrical and optical potentiation, and long-term optical potentiation in a single device. Neuromorphic behavior is demonstrated through spike-number-dependent plasticity under gate-voltage pulses and through the transition from short-term to long-term plasticity by increasing the power and number of optical pulses from a blue-light excitation. The device provides both electrical and optical outputs, measured as drain current and electroluminescence, respectively, making it promising for interfacing optical neural networks and neuromorphic sensing applications.

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Multifunctional Organic PhotoTransistor: Integrating Volatile and Non-Volatile Memory in a Single Device

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Artificial neural networks rely on the interplay between signal integration and memory, typically implemented through complex circuit architectures with significant computational overhead. [1] The development of device-level elements capable of simultaneously reproducing these functions offers a route toward more compact neuromorphic systems. [2] Organic electronic devices provide a versatile platform for this purpose; however, most approaches still rely on separate components or multi-device configurations to emulate neuron- and synapse-like behavior. [3] Here, we address this limitation by developing an organic phototransistor (OPT) that integrates both functionalities within a single device. The device is based on a hybrid dielectric architecture combining a relaxor-like ferroelectric polymer, poly(vinylidenefluoride-trifluoroethylene-chlorofluoroethylene) (PVDF-TrFE-CFE), and an optically modulated dielectric layer composed of poly(methyl methacrylate) (PMMA) and the persistent radical (3,5-dichloro-4-pyridyl)bis(2,6-dichloro-4-phenylphenyl)methyl radical (PyPBTM). [4,5] This system exhibits distinct neuromorphic functionalities depending on the stimulation mode. Under electrical excitation, it shows spike-number-dependent plasticity (SNDP) and paired-pulse facilitation (PPF), corresponding to short-term potentiation (STP), while enabling a leaky integrate-and-fire response with reversible relaxation to a stable baseline (maintained over ≥100 cycles). Under optical excitation (405 nm), it instead displays long-term potentiation (LTP), resulting in a stable, history-dependent modulation of the channel conductance, characteristic of synaptic weight storage. The coexistence of electrically driven STP and optically induced LTP within a single device demonstrates the feasibility of implementing both neuron-like and synapse-like functions at the device level. This approach provides a compact platform for simplified neuromorphic hardware and supports the development of integrated artificial neural networks and neuromorphic vision systems.

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Molecular Engineering of Side-Chains in Conjugated Polymers for Organic Memristors

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Abstract: Memristors, recognized as the fourth fundamental passive circuit element, represent a promising technology for linking electrical charge and variable resistance to retain memory [1]. Due to their significant potential in neuromorphic engineering and low-power computing, current research focuses on organic materials that offer high mechanical flexibility and tunable electronic properties through precise structural modification [2]. This work investigates a series of conjugated polymers based on dithieno[3,2-b:2′,3′-d]pyrrole (DTP) featuring varying alkyl chain lengths. The monomers were synthesized via palladium-catalyzed amination and subsequently electrochemically deposited to form stable thin films. Electronic characterization through cyclic voltammetry, spectroscopy, and computational modeling indicates that while the side-chain length has a negligible impact on the monomeric energy levels, the process of polymerization leads to a significant narrowing of the energy gap and a stabilization of the frontier molecular orbitals. Fabricated two-terminal devices exhibit robust, frequency-dependent pinched hysteresis loops. The most pronounced memristive response is observed in the low-frequency regime, where ion diffusion within the polymer bulk is most effective. Beyond basic switching, the devices successfully emulated fundamental biomimetic synaptic functions, including potentiation and depression. Under repetitive voltage pulse stimulation, the memristors demonstrated a gradual and reproducible modulation of electrical conductance. Comparative analysis reveals that the length of the alkyl substituents significantly influences the current densities and the sharpness of the switching dynamics. These findings suggest that while the conjugated backbone dictates the core optoelectronic properties, the side-chains facilitate the supramolecular environment necessary for efficient ion transport [3]. This study confirms that side-chain engineering is an effective strategy for tuning the response of organic memristors for future applications in advanced AI hardware and biosensing.

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Molecular Control of Polaron Formation and Transport in Organic Electrochemical Devices

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Polarons form when injected charges strongly couple to molecular vibrations in organic semiconductors, directly influencing charge transport and device operation. In organic electrochemical devices, such as organic electrochemical transistors (OECTs) and organic synaptic transistors (OSTs), ions further drive polaron formation, structural deformation, and charge localisation/delocalisation. However, direct in situ evidence linking ion-induced polarons to molecular structural changes and device function remains limited. In this talk, I will present our recent spectroscopic studies of conjugated polymers under electrochemical doping and gate-pulse operation. I will show how subtle side-chain changes, including alkyl/glycol chemistry and side-chain density, regulate polaron formation; how backbone extension modifies polaron delocalisation and transport; and how molecular structure controls ion retention during synaptic gate-voltage pulses. These results provide direct evidence of ion-coupled polaron formation and reveal how electron-phonon coupling governs charge transport, structural response, and memory behaviour in organic electrochemical devices.

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Epitaxy Meets Transfer Printing: A Pathway towards Organic Semiconductor Device Integration

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Organic semiconductors (OSCs) in thin-film form typically suffer from structural disorder that limits their optoelectronic performance. While organic epitaxy yields films whose properties approach those of single crystals, the substrates enabling epitaxial growth are incompatible with device integration – a key bottleneck for practical applications.

To overcome this limitation, we present a transfer printing (TP) method that relocates epitaxially grown OSC films from their native substrates to device-compatible ones,[1] while also decoupling interface engineering from the requirements of epitaxial growth. Our strategy harnesses the water solubility of organic crystalline substrates commonly used for epitaxial growth in combination with a polydimethylsiloxane (PDMS) stamp, enabling deterministic, orientation-controlled placement of crystalline films without protective resins or direct water exposure of the receiving substrate.

We demonstrate the method using rubrene films grown by organic molecular beam epitaxy on β-alanine single crystals.[2] The transferred films fully retain their morphology, crystalline orientation, anisotropic optical response, and photoluminescence dynamics – including the power-law triplet–triplet fusion kinetics characteristic of highly crystalline rubrene – as confirmed by AFM, XRD, polarization spectroscopy, and time-resolved PL. Notably, their optical properties remain stable after months of air storage.

Altogether, this work establishes a versatile platform for integrating epitaxially grown OSC films into functional device architectures, enabling full exploitation of the superior properties that epitaxy affords. Additional examples of transfer-printable organic semiconductors are also presented, further demonstrating the broad applicability of the method.

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Engineering Light with Defects: Vacancy-Driven Optical and Catalytic Functions in g-C_3N_4

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Graphitic carbon nitride (g−C_3N_4) is a metal-free semiconductor of great promise for sustainable photocatalysis,[1] whose performance can be enhanced with defect engineering, typically introducing nitrogen vacancies.[2] To fill this gap, we here present a study employing advanced first-principles simulations[3] to investigate the structural and electronic properties of nitrogen vacancies in monolayer g−C_3N_4, explicitly accounting for out-of-plane corrugation and supercell-size effects.

We show that the correct energetics of nitrogen vacancies can only be captured when long-range buckling of the g−C_3N_4 sheet is fully described.[4] Our analysis mainly focuses on two non-equivalent nitrogen vacancies, achieved upon removal of a N atom from either the center or the edge of the heptazine unit. Both are found to introduce localized in-gap states associated with shallow acceptor levels and deep donor levels. These are found to be related to the red-shifted absorption and weak photoluminescence observed experimentally for N-deficient g−C_3N_4 samples.

Furthermore, energy-level alignment of the defects states at the water-semiconductor interface provides a rationale for the experimentally reported enhancement of photocatalytic reduction reactions, concomitant with a deterioration of oxidation activity. Overall, our study establishes direct correspondences between defect-induced electronic structure modifications and multiple experimental observables, offering a unified microscopic framework that connects nitrogen-vacancy physics to the photocatalytic and optoelectronic properties of g-C3N4, and provides a transferable, predictive strategy for the rational design and discovery of defect-engineered carbon nitride photocatalysts and related metal-free catalytic materials.[4]

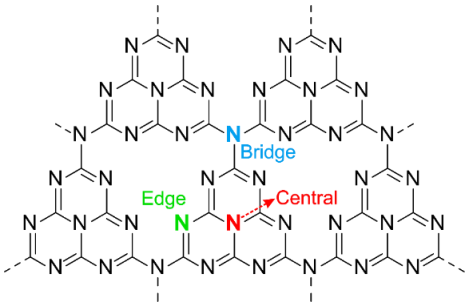

Fig. 1: g−C_3N_4 structure with defects highlighted.

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