16th European Conference on Molecular Electronics

2 - 6 October 2023
Bari, Italy

BARI
ECME 2023
BARI - ITALY 2 - 6 OCTOBER

ABSTRACT BOOK

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ECME 2023

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16th European Conference of Molecular Electronics (ECME)

Bari, Italy | October 2-6, 2023

Municipal Theatre Niccolò Piccinni

Conference Website: https://www.ecme2023.eu/

Welcome to ECME 2023: Advancing the Frontiers of Molecular Electronics

It is with great pleasure that we welcome you to the 16th European Conference of Molecular Electronics (ECME), which is held in the picturesque city of Bari, Italy. ECME, renowned as the premier European conference in the realm of Molecular Electronics, has a rich history of fostering interdisciplinary discussions, knowledge exchange, and collaborative endeavors. The 2023 edition of ECME promises to uphold this esteemed tradition and further propel the field to new heights.

A Legacy of Excellence

The ECME series of conferences held every two years has been held in various European cities over the years, symbolizing the unity of minds across borders. From its inception in Padua, Italy, in 1992, to its most recent gathering in Linköping, Sweden, in 2019, ECME has consistently attracted leading scientists, researchers, and experts in the fields of chemistry, physics, biology, materials science, nanoscience, engineering, devices, and commercialization. The conference's rich history includes stops in Germany, Belgium, the UK, the Netherlands, France, and Denmark, each contributing invaluably to knowledge and innovation.

A Multidisciplinary Exploration

ECME 2023 promises to be a dynamic and interdisciplinary platform that transcends traditional boundaries. Delegates will delve into a wide choice of topics encompassing molecular-organic and plastic electronics. From fundamental research to practical applications, our conference will address the entire spectrum of molecular electronics, stimulating intellectual curiosity and sparking ideas.

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Discover Bari: A Cultural Gem

Beyond the stimulating scientific program, ECME 2023 offers attendees the opportunity to immerse themselves in the rich cultural tapestry of Bari, the capital of the Apulia region. The conference venue, the Municipal Theatre Niccolò Piccinni, is ideally located in the heart of the city, directly connected to the international airport, and a stone's throw away from the medieval quarter known as "Bari Vecchia." Explore the city's historic landmarks, medieval churches, and captivating art and architecture. Stroll along Bari's spectacular promenade, which overlooks the crystal-clear sea and is within walking distance of the conference venue.

Culinary Delights of Bari

While in Bari, delegates can savor the delectable local cuisine served in the city's cousy restaurants, trattorias, and osterias. The Delegates should not miss the opportunity to indulge in Bari's renowned street food, including the irresistible focaccia and panzerotti.

In conclusion, ECME 2023 promises not only to be a catalyst for scientific progress but also an unforgettable cultural experience. We extend our warmest invitation to you to be a part of this exceptional gathering of minds, fostering collaborations and advancing the frontiers of Molecular Electronics.

For more details about the conference, please visit our official website at https://www.ecme2023.eu/.

We look forward to welcoming you all at ECME 2023 in Bari, Italy.

Warm regards,
Luisa Torsi and Gianluca Maria Farinola
ECME 2023 Chairpersons

UniBa Università degli Studi di Bari Aldo Moro Politecnico di Bari Società Chimica Italiana Comune di Bari REGIONE PUGLIA

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Official Conference Guide

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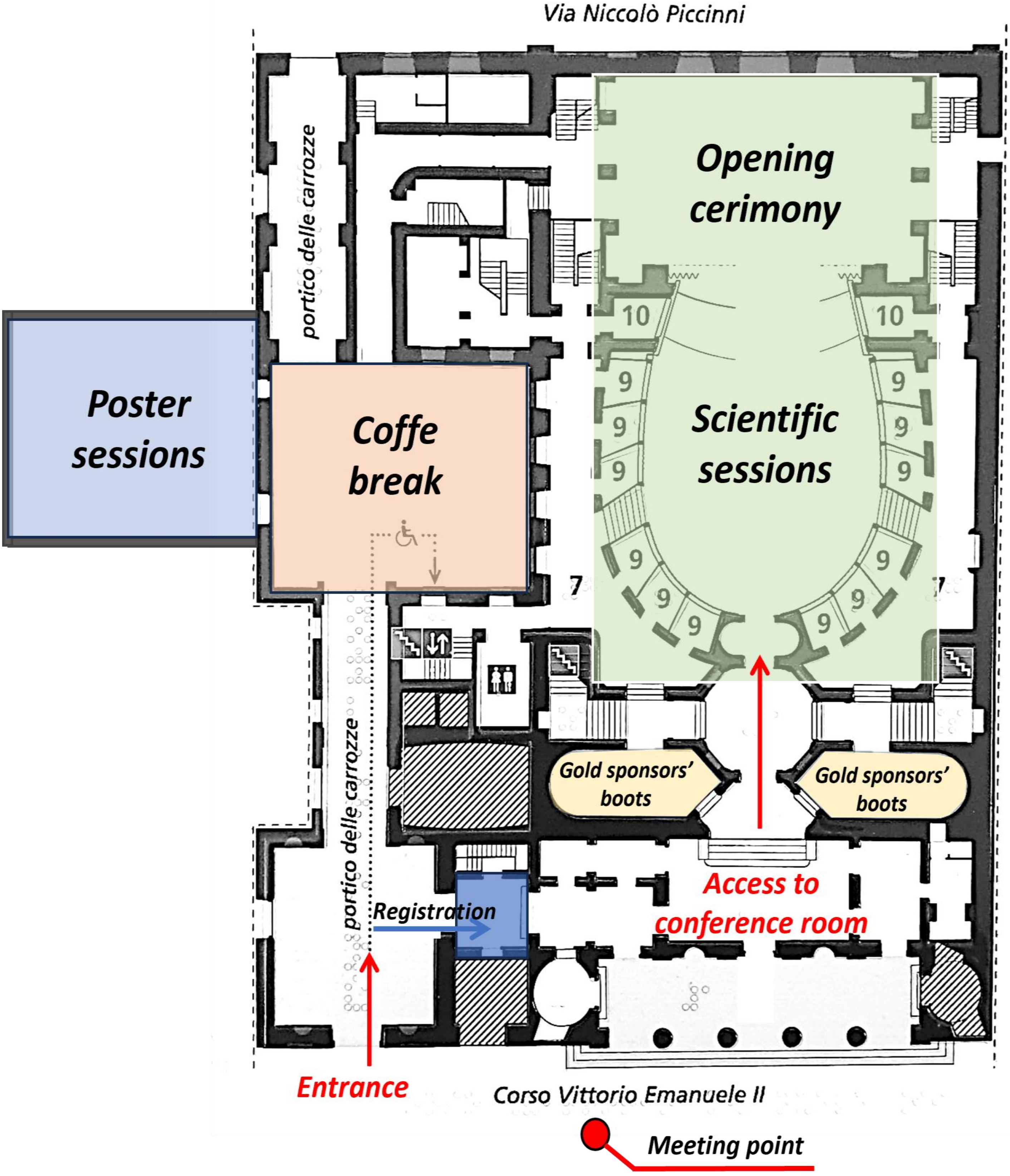
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Program of the Conference
Piccinni Theatre
Corso Vittorio Emanuele II, 84,
70122 - Bari BA – Apulia - Italy

Sunday, October, 1st 2023	
17:00-18:00	Registration
18:00-20:00	**Welcome party - Museo Archeologico di Santa Scolastica**

Monday, October, 2nd 2023			
08:30-09:30	Opening Cerimony		
09:30-10:50	**Session 1A - Chair: Gianluca Maria Farinola**		
09:30-10:00	**PL 1.1**	Fabio Biscarini	Physico-Chemical insights on Organic Electronics Biosensors
10:00-10:20	**KL 1.1**	Guglielmo Lanzani	Intra Membrane Light actuators for Cell Photostimulation
10:20-10:35	Oral 1.1	Serpil Tekoglu	Conductive Biocomposites for Biomedical Applications
10:35-10:50	Oral 1.2	Fabrizio Torricelli	Organic Artificial Neurons for in-situ Bioelectronics
10:50-11:20	Coffee Break & Poster Preview		
11:20-13:00	**Session 1B - Chair: Georges Hadziioannou**		
11:20-11:40	**KL 1.2**	Roisin Owens	Bioelectronic tools to study the gut-brain axis
11:40-12:00	**KL 1.3**	Ifor Samuel	Approaches to Electrically Driven Organic Semiconductor Lasers
12:00-12:15	Oral 1.3	Hübler Arved	Print the Brain: Neuromorphic 3D-Circuits Based on Printed Organic Memristors

12:15-12:30	Oral 1.4	Adrica Kyndiah	Direct Recording of Action Potentials of Cardiomyocytes Through Printed Electrolyte-Gated Field-Effect Transistors
12:30-12:45	Oral 1.5	Maria Rosa Antognazza	Cell mechanotransduction driven by bio-organic optoelectronic devices
12:45-13:00	Oral 1.6	Giuseppe M. Paternò	Membrane Targeted Azobenzene Drives Optical Modulation of Bacterial Membrane Potential
13:00-14:00	Free Time		
14:00-15:55	**Session 1C - Chair: Gitti Frey**		
14:00-14:30	**PL 1.2**	Antonio Facchetti	Unconventional semiconductors and device architectures enabled by molecular design, doping and film morphology engineering
14:30-14:50	**KL 1.4**	Natalie Stingelin	Flexible Electronics: Challenges and Opportunities — a Materials Science View
14:50-15:10	**KL 1.5**	Christoph Brabec	Towards A Digital Twin for Organic and Perovskite Photovoltaics
15:10-15:25	Oral 1.7	Tianjun Liu	Chiral emission from halide perovskite semiconductors
15:25-15:40	Oral 1.8	Ning Li	Mastering morphology of non-fullerene acceptors towards long-term stable organic solar cells
15:40-15:55	Oral 1.9	Andrea Nitti	Organic Electronic Materials via Cascade Synthetic Approach based on One Pot DHA-Perkin Annulations
15:55-16:20	Coffee Break & Poster Preview		
16:20-17:50	**Session 1D - Chair: Roisin Owens**		
16:20-16:35	Oral 1.10	Guido Fratesi	Metal-TetraPhenyl-Porphyrins Adsorption on Atom-Thick and Bulk Magnetic Oxides
16:35-16:50	Oral 1.11	Marta Penconi	Paradigm Shift in Iridium Emitters Structure: Single Active Ligand in Heteroleptic Complexes for NIR Phosphorescent OLEDs
16:50-17:05	Oral 1.12	Chloè Dindault	Organic Photodetectors and their tolerance to impurities
17:05-17:20	Oral 1.13	Yunzhou Deng	Excitation “memory” accelerates transient electroluminescent response of quantum-dot lightemitting diodes
17:20-17:35	Oral 1.14	Silvia Colella	Chemical insight into perovskite inks behaviour and their implications in photovoltaic devices
17:35-17:50	Oral 1.15	Elena Molteni	Tuning the magnetic properties of antiferromagnetic oxides via adsorption of organic molecules: pentacene on NiO(001)
17:50-19:30	**Poster Session 1: tasting of Peroni brewery beers and Apulian taralli**		

Tuesday, October, 3rd 2023

09:00-10:50	**Session 2A - Chair: Maurizio Prato**		
09:00-09:30	**PL 2.1**	Takao Someya	Electronic skins for robotics and wearables
09:30-09:50	**KL 2.1**	Annalisa Bonfiglio	Double-gated organic transistors for biomedical sensing applications: overall analysis and future perspectives.
09:50-10:05	Oral 2.1	Alessandro Luzio	Copper Phthalocyanine Based Electrochemical Transistors for Future Edible Electronics
10:05-10:20	Oral 2.2	Yan Wang	Permeable electronic skins for health monitoring
10:20-10:35	Oral 2.3	Francisco Molina-Lopez	2D/3D-Printed Flexible Organic Thermoelectrics for LowScale Energy Harvesting
10:35-10:50	Oral 2.4	Eyal Stein	Ambipolar Blend-based Organic Mixed Ionic-Electronic Conductors
10:50-11:20	Coffee Break & Poster Preview		
11:20-13:00	**Session 2B - Chair: Nuria Crivillers**		
11:20-11:40	**KL 2.2**	Fei Huang	High Performance n-Type Conjugated Polymers for Organic Electronics
11:40-12:00	**KL 2.3**	Iain McCulloch	Organic Semiconducting Polymer Photocatalysis for Water and CO2 Reduction
12:00-12:15	Oral 2.5	Cloutet Eric	Synthesis of (semi)conducting polymers in dispersed media
12:15-12:30	Oral 2.6	Theresa Rienmüller	Modeling cellular membrane potential using organic photovoltaic devices
12:30-12:45	Oral 2.7	Jozef Krajcovic	Side chain engineering: the role of bulky substituents towards to original properties of organic optoelectronic materials
12:45-13:00	Oral 2.8	Johannes Gierschner	Charge Transfer State Engineering for Tailor-Made Luminescent Organic Materials
13:00-14:00	Free Time		
14:00-16:10	**Session 2C - Chair: Antonio Facchetti**		
14:00-14:30	**PL 2.2**	Magnus Berggren	Substrate-free Organic Bioelectronics Integrated with Living Cells and Tissues
14:30-14:50	**KL 2.4**	Eleni Stavrinidou	Plant bioelectronics for high resolution monitoring and electronic control of plant processes
14:50-15:05	Oral 2.9	Mingna Liao	Cellulose-Based Radiative Cooling and Solar Heating Powers Ionic Thermoelectrics
15:05-15:20	Oral 2.10	Stephanie Valianti	Charge-Transport Mechanisms in Desulfobubaceae Microbial Nanowires (Cable Bacteria)
15:20-15:35	Oral 2.11	Matteo Grattieri	Bio-inspired Approaches for Biotic/abiotic Interfaces in Intact Bacteria-based Biophotoelectrochemical Systems
15:35-15:50	Oral 2.12	Marianna Ambrico	Mixing and matching sustainable Melanin&Keratin from waste for green electronics
15:50-16:30	Coffee Break & Poster Preview		

16:30-18:00	**Session 2D - Chair: Magnus Berggren**		
16:30-16:45	Oral 2.13	Arianna Magni	The Photophysics of Cell Membrane-Targeting Phototransducers
16:45-17:00	Oral 2.14	Fabio Marangi	On the Coupling Mechanism Occurring at the Neuron-Nanoparticle Interface
17:00-17:15	Oral 2.15	Elliot Goldberg	The Effects of Strain on the Electronic Properties of Rubrene Single Crystals
17:15-17:30	Oral 2.16	Giuseppina Pace	2D-Materials and Hydrogels based Triboelectric Nanogenerators (TENGs) for Energy Harvesting and Self-Powered Tactile Sensors
17:30-17:45	Oral 2.17	Arianna Quesada Ramirez	Ellipsometric measurements in organic semiconducting materials for photovoltaics
17:45-18:00	Oral 2.18	Hang Yu	Towards a Deeper Understanding of the Ionic Charging in Naphthalenediimide-Based N-Type Conjugated Polymer Electrodes
18:00-19:30	**Poster Session 2: tasting of Peroni brewery beers and Apulian taralli**		

Wednesday, October, 4th 2023

09:00-10:50	**Session 3A - Chair: Alberto Salleo**		
09:00-09:30	**PL 3.1**	Paolo Samorì	Supramolecular opto-electronics: digital multiresponsive devices with enhanced functionalities
09:30-09:50	**KL 3.1**	Maurizio Prato	Synthesis, Properties and Applications of Carbon Nanodots
09:50-10:05	Oral 3.1	Chris McNeill	Resonant Tender X-ray Scattering of Conjugated Polymers
10:05-10:20	Oral 3.2	Michal Valasek	Electrically and mechanically decoupled single chromophores by tripodal scaffolds on gold: Towards Organic Optoelectronic Devices
10:20-10:35	Oral 3.3	Giovanni Costantini	Quantitative characterisation of conjugated polymers: mass distribution and polymerisation defects determined by molecular scale imaging
10:35-10:50	Oral 3.4	Edmund Leary	How Does Antiaromaticity Affect Single Molecule Conductance?
10:50-11:20	Coffee Break		
11:20-13:25	**Session 3B - Chair: Fabio Biscarini**		
11:20-11:50	**PL 3.2**	Thuc-Quyen Nguyen	Conjugated Polyelectrolytes for Opto-electronic Devices
11:50-12:10	**KL 3.2**	Feng Gao	Minimizing voltage losses in organic solar cells
12:10-12:25	Oral 3.5	Ergang Wang	Non-Conjugated Polymeric and Dimeric Acceptors for Efficient Polymer Solar Cells
12:25-12:40	Oral 3.6	Mathias Nyman	Controlled Doping of the Active Layer as a possible Performance Enhancer in Organic Solar Cells
12:40-12:55	Oral 3.7	Chang-Qi Ma	Degradation Mechanism and Stability Improvement of Organic Solar Cells
12:55-13:10	Oral 3.8	Jeannine Grune	Triplet excitons and associated efficiency-limiting pathways in organic photovoltaics based on non-fullerene acceptors
13:10-13:25	Oral 3.9	Ramesh Y. Adhikari	Transparent Conductive Films of PEDOT:PSS-Amino Acid Composite
13:25-14:30	Lunch Buffet		
15:00	Transfer to Alberobello, meeting point Teatro Piccinni		
16:15-19:00	Alberobello Tour		
19:30	Transfer from Alberobello to Social Dinner		
20:00-23:00	Social Dinner: Masseria Agriturismo Lama San Giorgio		

Thursday, October, 5th 2023

09:00- 10:50	**Session 4A - Chair: Thuc-Quyen Nguyen**		
09:00- 09:30	**PL 4.1**	Alberto Salleo	Do crystals matter in conjugated polymers? Linking microstructure to charge transport at several length scales
09:30- 09:50	**KL 4.1**	Marta Mas Torrent	Towards reproducible, stable and reliable printed OFETs
09:50- 10:05	Oral 4.1	Natalie Banerji	Terahertz Spectroscopy as a Tool to Study Charge Carriers in Functional Organic Semiconductors
10:05- 10:20	Oral 4.2	Pia Damlin	Probing the electronic and structural properties of organic flexible thin films by in situ spectro-electrochemistry
10:20- 10:35	Oral 4.3	Regina Hoffmann-Vogel	Shell effects in electromigrated Cu-nanocontacts under ambient conditions
10:35- 10:50	Oral 4.4	Tae-il Kim	Choline ion gel based organic electrochemical transistors for bioelectronics
10:50- 11:20	Coffee Break & Poster Preview		
11:20- 13:00	**Session 4B - Chair: Guglielmo Lanzani**		
11:20- 11:40	**KL 4.2**	Maria Antonietta Loi	SnO_2 for inverted non-fullerene acceptor organic solar cells
11:40- 12:00	**KL 4.3**	Dirk Guldi	Adaptive Down- and Up-Conversion
12:00- 12:15	Oral 4.5	Fengling Zhang	Investigate the Effect of Solvent and Additive in Formation of All-Polymer Solar Cells with Situ Optical Spectroscopy
12:15- 12:30	Oral 4.6	Daniela De Venuto	A Wearable and Flexible Potentiometric Chloride Activity Sensing Platform with Replaceable Electrodes for Cystic Fibrosis Diagnosis at home
12:30- 12:45	Oral 4.7	Peter Baeuerle	Molecular Donor-Acceptor Dyads and Triads for Single Material Organic Solar Cells
12:45- 13:00	Oral 4.8	Nuria Crivillers	Photoluminescence properties of single-walled carbon nanotubes modified with Stable Organic Radicals
13:00- 14:00	Free Time		
14:00- 16:05	**Session 4C - Chair: Zhenan Bao**		
14:00- 14:30	**PL 4.2**	Takuzo Aida	Electronically or Electrically Active Dynamic Materials Based on Supramolecular Polymers
14:30- 14:50	**KL 4.4**	Yoann Olivier	Controlling spin by materials design in light-emitting applications: A computational perspective
14:50- 15:05	Oral 4.9	Xianjie Liu	Optoelectronic properties of two-dimensional organic molecular crystals upon their electronic structure
15:05- 15:20	Oral 4.10	Elena Mena-Osteritz	Toroidal Through Space Conjugation in 3D-Aromatic Molecules
15:20- 15:35	Oral 4.11	Alberto Bossi	3D Supramolecular Hybrid Heterostructures on Highly Ordered 2D Thin Film: Coordination Chemistry at Work with Tetrapyrrolic Macrocycles Network
15:35- 15:50	Oral 4.12	Kai Lin Woon	Fast and Accurate Determination of the Singlet–Triplet Gap in Donor–Acceptor and Multiresonance TADF Molecules by Using Hole–Hole Tamm–Dancoff Approximated Density Functional Theory

15:50-16:05	Oral 4.13	Daniele Padula	Identification of Unknown Inverted Singlet-Triplet Cores by High--Throughput Virtual Screening
16:05-16:30	Coffee Break & Poster Preview		
16:30-18:00	**Session 4D - Chair: Marta Mas**		
16:30-16:45	Oral 4.14	Alessandro Landi	Simulation of organic mixed ionic and electronic conductors with a combined classical and quantum mechanical model
16:45-17:00	Oral 4.15	Tahereh Nemetiaram	Organic Electronics from Structural Database: New High Mobility Materials and Design Strategies
17:00-17:15	Oral 4.16	Wei Wu	Integrated simulation of organic materials: From stationary to dynamical
17:15-17:30	Oral 4.17	Hesam Makki	High-throughput modelling of semiconducting polymers: a revolutionary route to in silico design of conjugated polymer
17:30-17:45	Oral 4.18	Wenlan Liu	An *ab initio* method on predicting absorption spectra of crystalline organic semiconducting films
17:45-18:00	Oral 4.19	Thomas Baschè	Boosting the Fluorescence Yield of a NIR Quantum Emitter
18:00-19:30	**Poster Session 3: tasting of Peroni brewery beers and Apulian taralli**		

Friday, October, 6th 2023

09:00-10:45	**Session 5A - Chair: Luisa Torsi**		
09:00-09:30	**PL 5.1**	Zhenan Bao	Skin-inspired organic electronics
09:30-09:45	Oral 5.1	Stefano Toffanin	Organic Optoelectronic Components in a Smart-integrated System for Plasmonic-based Sensing
09:45-10:00	Oral 5.2	Stefano Casalini	Sustainable manufacturing of reduced-graphene oxide electrolyte-gated transistors: characterization, understanding and applications
10:00-10:15	Oral 5.3	Cinzia Di Franco	Kelvin-probe force microscopy of surface potential shift triggered by affinity binding in large-area bio-functionalized surfaces
10:15-10:30	Oral 5.4	Gabriel Gomila	Multiparametric nanocharacterization of electrolyte gated organic transistors in operando
10:30-10:45	Oral 5.5	Sabrina Steffens	Contact Resistance of Low-Voltage n-Channel Thin-Film Transistors Based on Three Different Organic Semiconductors
10:45-11:15	Coffee Break		
11:15-12:45	**Session 5B - Chair: Eleonora Macchia**		
11:15-11:30	Oral 5.6	Mario Barra	Ambipolar transport and space-charge accumulation effects in organic heterojunction field-effect transistors
11:30-11:45	Oral 5.7	Ilary Belardi	Brewer’s spent grain for greener OTFT structures
11:45-12:00	Oral 5.8	Li Changbai	Printed Bioelectronics via In-Situ Enzymatic Polymerization of Conjugated Oligomer-based Hydrogel Bioinks
12:00-12:15	Oral 5.9	Hela Fadool	Enhancing the Performance of State-of-Art solar cells by improving the Built-in Potential
12:15-12:30	Oral 5.10	Davide Vurro	Printed Wearable Electronics for Healthcare
12:30-13:15	Closing Cerimony		

Plenary speakers

PL 1.1

Physico-Chemical insights on Organic Electronics Biosensors

Prof. Fabio Biscarini

UNIMORE Università degli Studi di Modena e Reggio Emilia

Fabio Biscarini is Full Professor of Chemistry at University of Modena and Reggio Emilia (UNIMORE) and Senior Researcher at the Center for Translational Neurophysiology-IIT in Ferrara, where he heads the research line “Organic Neuroelectronics”.

His research interests are organic bioelectronics, label-free biosensors, implantable devices for bidirectional communication with the brain, organic neuromorphic devices.

PL 1.2

Unconventional semiconductors and device architectures enabled by molecular design, doping and film morphology engineering

Antonio Facchetti

Adjunct Professor at Northwestern University

Antonio Facchetti is aAdjunct Professor at Northwestern Universityn Adjunct Professor at Northwestern University. He has published about 560 research articles and holds about 120 patents. He received the ACS Award for Creative Invention, the Giulio Natta Gold Medal and he is a Fellow of the EAS, NAI, MRS, AAAS, PMSE, Kavli, and RSC.

PL 2.1

Electronic skins for robotics and wearables

Takao Someya

Professor, Graduate School of Engineering The University of Tokyo

Takao Someya is Professor at the University of Tokyo and Chief Scientist at RIKEN. His expertise is stretchable and organic electronics, developing the world's first stretchable electronic skin for robotic application. He also conducted research at Columbia University and Bell Labs and is currently VP of the Material Research Society.

PL 2.2

Substrate-free Organic Bioelectronics Integrated with Living Cells and Tissues

Magnus Berggren

Linköping University

In 1991 he received a master’s degree in physics and in 1996 a doctoral degree in physics at Linköping University. He then joined Bell Laboratories in the United States, for a one-year post doc research period. In 2001 he was appointed as a professor of organic electronics at Linköping University.

His research addresses how to utilise organic electronics in novel applications such as in printed-paper electronics and in biology applications. Magnus Berggren Magnus Berggren wins Wallenberg prize LiU News News events

In 2011 Magnus Berggren became an elected member of the Royal Swedish Academy of Sciences. Since 2005 he has been the Director of the Strategic Research Centre for Organic Bioelectronics, OBOE, at Linköping University, which is funded by the Swedish Foundation for Strategic Research.

PL 3.1

Supramolecular opto-electronics: digital multiresponsive devices with enhanced functionalities

Paolo Samorì

Professor at the Université de Strasbourg and Director of the Institut de Science et d'Ingénierie Supramoléculaires.

Paolo Samorì is Distinguished Professor at the Université de Strasbourg and Director of the Institut de Science et d'Ingénierie Supramoléculaires. His research interests comprise nanochemistry, materials chemistry and supramolecular sciences with a specific focus on 2D materials and functional organic/polymeric and hybrid nanomaterials for application in optoelectronics, energy and sensing.

PL 3.2

Conjugated Polyelectrolytes for Opto-electronic Devices

Thuc-Quyen Nguyen

Professor of Chemistry and Biochemistryat University of California, Santa Barbara (UCSB)

Thuc-Quyen Nguyen is the Director of the Center for Polymers and Organic Solids and professor in the Department of Chemistry & Biochemistry at the University of California, Santa Barbara (UCSB). Her research interests are doping and charge transport in organic semiconductors, bioelectronics, and device physics of organic solar cells, ratchets, transistors, and photodetectors.

PL 4.1

Do crystals matter in conjugated polymers?

Linking microstructure to charge transport at several length scales

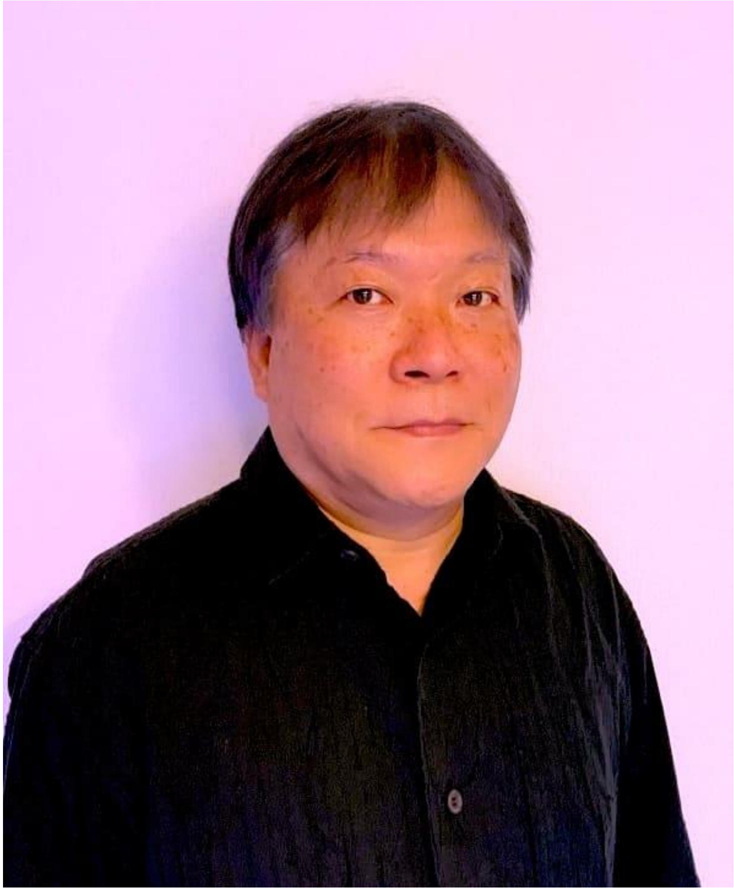
Alberto Salleo

Professor of Materials Science and Department Chair at Stanford University

Alberto Salleo is Professor of Materials Science and Department Chair at Stanford. Salleo is a Clarivate Highly Cited Researcher since 2015, he was elected to the European Academy of Sciences in 2021 and is Fellow of the MRS since 2022.

PL 4.2

Electronically or Electrically Active Dynamic Materials Based on Supramolecular Polymers



Takuzo Aida

University of Tokyo

Prof. Aida was born in 1956 in Oita (Japan). He received the Ph.D. in Polymer Chemistry at the University of Tokyo in 1984, being awarded the Inoue Research Award for Young Scientists for research on precision macromolecular synthesis based on metalloporphyrin complexes. After being appointed as an Assistant Professor in the Department of Synthetic Chemistry at the University of Tokyo, he was visiting researcher at the IBM Almaden Research Center. He became Associate Professor in 1991 and Full Professor in the Department of Chemistry and Biotechnology at the University of Tokyo in 1996. Prof. Aida also served as a researcher in the Japan Science and Technology Agency (JST) and he was appointed as visiting Professor at the Institute for Molecular Science in Okazaki.

He is currently the Deputy Director for the RIKEN Center for Emergent Matter Science (CEMS) and Distinguished University Professor at the University of Tokyo.

Prof. Aida is recognized for his pioneering contribution in the field of Supramolecular Chemistry, combining basic knowledges of Organic Chemistry with Macromolecular Science, Photochemistry and Electrochemistry. Besides his fundamental contributions to the understanding of supramolecular systems, he has promoted their widespread use by developing materials for a variety of applications, ranging from optoelectronics to catalysis, bio-related molecular recognition and production of environmentally friendly organic materials.

PL 5.1

Skin-inspired organic electronics

Zhenan Bao

K.K. Lee Professor of Chemical Engineering, and by courtesy, a Professor of Chemistry and a Professor of Material Science and Engineering at Stanford University

Bao directs the Stanford Wearable Electronics Initiate (eWEAR) since 2016. Prior to joining Stanford in 2004, she was a Distinguished Member of Technical Staff in Bell Labs, Lucent Technologies from 1995-2004. She received her Ph.D in Chemistry from the University of Chicago in 1995. She has over 700 refereed publications and over 100 US patents with a Google Scholar H-Index >195. She is one of the Clarivate Citation Laureates. Bao is a member of the National Academy of Engineering, the American Academy of Arts and Sciences and the National Academy of Inventors. She a foreign member of the Chinese Academy of Science.

Keynote speakers

KL 1.1

Intra Membrane Light actuators for Cell Photostimulation

Guglielmo Lanzani

Department of Physics

Politecnico di Milano

KL 1.2

Bioelectronic tools to study the gut brain axis

Roisin Owens

Department of Chemical Engineering and Biotechnology

University of Cambridge

KL 1.3

Approaches to Electrically Driven Organic Semiconductor Lasers

Ifor Samuel

Organic Semiconductor Centre, School of Physics and Astronomy

University of St Andrews

KL 1.4

Flexible Electronics: Challenges and Opportunities a Materials Science View

Natalie Stingelin

Professor and Chair, School of Materials Science and Engineering Director, Center for Organic Photonics and Electronics (COPE)

School of Materials Science & Engineering, Georgia Institute of Technology, Atlanta, GA, U.S.A.

KL 1.5

Towards A Digital Twin for Organic and Perovskite Photovoltaics

Christoph Brabec

Department of Materials Science and Engineering Chair of Materials for Electronics and Energy TechnologyBiotechnology

i-MEET Institute Materials for Electronics and Energy Technology

KL 2.1

Double gated organic transistors for biomedical sensing applications: overall analysis and future perspectives.

Annalisa Bonfiglio

Professor of Bioengineering, formerly Chair Of The Board Of Directors presso CRS4 (Center for Advanced Studies, Research and Development in Sardinia)

Dept of Electrical and Electronic Engineering,University of Cagliari - Italy Scuola Universitaria Superiore IUSS - Pavia – Italy

KL 2.2

High Performance n Type Conjugated Polymers for Organic

Electronics

Fei Huang

Institute of Polymer Optoelectronic Materials and Devices

South China University of Technology

KL 2.3

Organic Semiconducting Polymer Photocatalysis for Water and CO2 Reduction

Iain McCulloch

Professor of Polymer Materials

University of Oxford

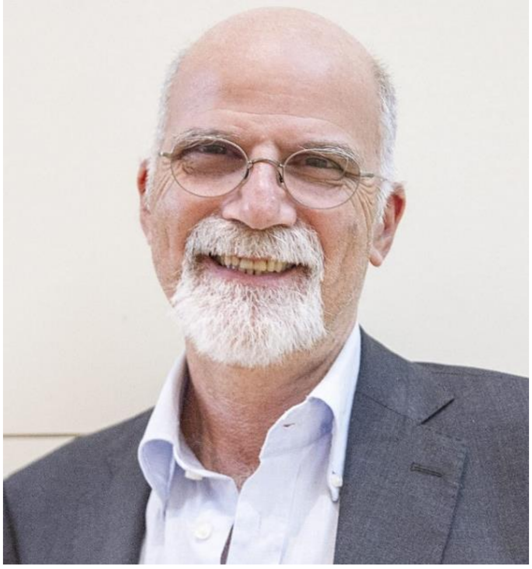
KL 2.4

Plant bioelectronics for high resolution monitoring and electronic control of plant processes

Eleni Stavrinidou

Department of Science and Technology (ITN)
Laboratory of Organic Electronics (LOE)

Linköping University



KL 3.1

Synthesis, Properties and Applications of Carbon Nanodots

Maurizio Prato

Ikerbasque Research Professor - AXA Research Professor Carbon Nanobiotechnology group - Center for Cooperative Research in Biomaterials San Sebastián, Spain

Department of Chemical and Pharmaceutical Science Università degli Studi di Trieste

KL 3.2

Minimizing voltage losses in organic solar cells

Feng Gao

Professor, Head of Unit Organic and perovskite semiconductors for energy technologies

Linköping University, Sweden

KL 4.1

Towards reproducible, stable and reliable printed OFETs

Marta Mas

CSIC Full Professor - Research Scientist Organic Electronics Materials and Devices

Institut de Ciència de Materials de Barcelona (ICMAB-CSIC)

KL 4.2

SnO2 for inverted non fullerene acceptor organic solar cells

Maria Antonietta Loi

Faculty of Science and Engineering Photophysics and OptoElectronics — Zernike Institute for Advanced Materials

University of Groningen

KL 4.3

Adaptive Down and Up Conversion

Dirk Guldi

Department of Chemistry and Pharmacy Chair of Physical Chemistry I

Friedrich Alexander University Erlangen-Nürnberg

KL 4.4

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

Yoann Olivier

NAmur Research College (NARC)

Universitè de Namur

Abstracts – oral contributions

O 1.1

Conductive Biocomposites for Biomedical Applications

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Conductive polymers such as poly(3,4-ethylenedioxythiophene):polystyrene sulfonate (PEDOT:PSS) are important components of soft and implantable bioelectronics[1]. Biocomposites, on the other hand, are materials that are composed of natural polymers and other materials, e.g., synthetic polymers. Natural biopolymers and their composites have attracted great attention for biomedical applications due to their biocompatibility, biodegradability, and low toxicity nature[2]. They can be utilized for a variety of applications, including drug delivery, tissue engineering, and medical implants[3].
One example of natural polymer that we investigated for bio- and organic electronics is deoxyribonucleic acid (DNA)[4-7], which is extracted from salmon fish residuals as a waste marine product[4]. **DNA** is an abundant polymer found in all organisms. The synthesized PEDOT:DNA and polypyyrole:DNA (PPy:DNA) biocomposites possess high biocompatibility toward cell culture without any significant cytotoxicity and electrical characteristics comparable to the commonly used PEDOT:PSS. A model transistor device with a channel material of novel biocomposites shows a moderate transconductance value, which can perform for bioelectronics[7]. As a follow up study, we focus on natural macromolecular polysaccharides such as **Sacran** (blue green algal polysaccharide) and **cellulose nanocrystals** to combine with PEDOT within novel biocomposites. A comprehensive study is performed with the synthesis, characterization, and properties of biocomposites and correlating them with their micro- and nanostructure. Overall, the implementation of natural polymers and biocomposites in medicine has the potential to revolutionize the field by providing safer, more effective treatments for a range of medical conditions.

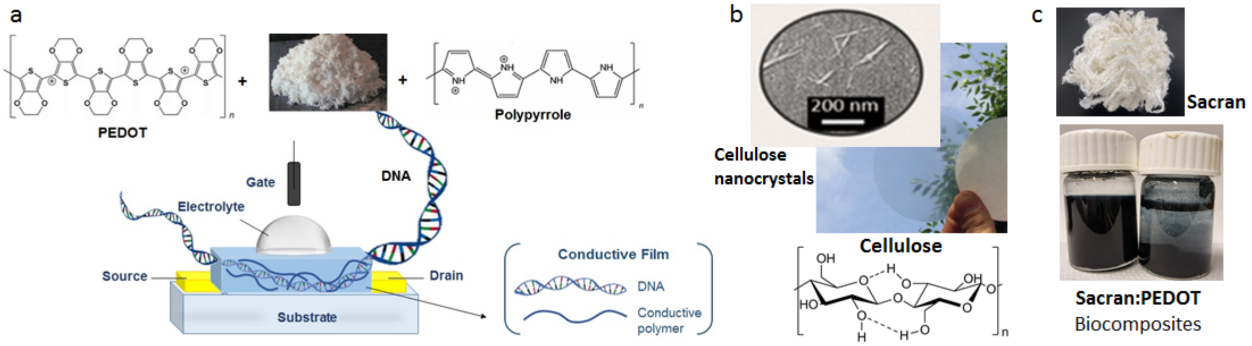

Figure: a) PEDOT:DNA and PPy:DNA as channel materials in electrochemical transistor architecture[7], b) SEM images of cellulose nanocrystals and cellulose chemical structure[8], c) PEDOT:Sacran colloidal solution.

References

[1] D.T. Simon, E.O. Gabrielsson, K. Tybrandt, M. Berggren, Chem. Rev. 116, 21, 13009–13041 (2016).
[2] S. Lee, S.M. Silva, L.M.C. Aguilar, T. Eom, S.E. Moulton, B.S. Shim, J. Mater. Chem. B, 10, 8575 (2022)
[3] C. Wang, T. Yokota, T Someya, *Chem. Rev.* 121, 4, 2109–2146 (2021).
[4] B. Singh, N. S. Sariciftci, J. Grote, F. Hopkins, J. of Appl. Phys. 100, 024514, (2006).
[5] C. Yumusak, B. Singh, N. S. Sariciftci, J. Grote, Appl. Phys. Lett. 95, 263304, (2009).
[6] S. Tekoglu, M. Held, M. Bender, G. Hernandez-Sosa et a. Adv. Sustainable Syst. 2000203 (2021).
[7] S. Tekoglu, D. Wielend, M. C. Scharber, N. S. Sariciftci, C. Yumusak, Adv. Mat. Tech. 1900699, (2020).
[8] A. Operamolla, C. Mazzuca, L. Micheli et al. ACS Applied Materials & Interfaces, 13, 44972 (2021).

O 1.2

Organic Artificial Neurons for in-situ Bioelectronics

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Neurons are the fundamental units of the nervous system and communicate with each other through synapses in a liquid environment. While conventional microelectronic approaches can mimic some aspects of neuronal behavior using oscillatory circuits [1], they result in bulky circuits that cannot operate in liquid environment and are not suitable for direct integration with biological systems [2]. Organic electrochemical devices based on organic mixed ionic–electronic conductors offer an alternative approach to neuromorphic electronics [3-5].

In this talk, we introduce an organic artificial spiking neuron (OAN) that offers local and in-situ neuromorphic sensing and biointerfacing. The OAN operates in a liquid and exhibits biosensing capabilities. It consists of a compact nonlinear electrochemical element with negative differential resistance that responds to the biological environment [6]. The OAN's spiking response is influenced by the ionic species commonly found in the extracellular space, and its behavior mimics that of a biological neuron surrounded by various biological carriers for signaling and processing.

The OAN shows stable spiking properties that depend on the local ionic, biomolecular, or neurotransmitter species present in the surrounding aqueous environment. Changes in ionic and biomolecular concentrations can modulate the neuronal excitability and trigger spikes. Ion-specific oscillations, particularly for sodium and potassium, which mimic ion channel dynamics are demonstrated. Moreover, we show the creation of a biohybrid interface where an artificial neuron interacts synergistically with membranes of epithelial cells. The biological membrane barrier can modulate the spiking properties of the artificial neuron in real time. The various functions of the OAN are discussed and investigated, to provide insights into the key mechanisms underlying the operation of the OAN. Overall, this research presents an organic artificial spiking neuron that offers control and sensing capabilities for neuromorphic applications and can be integrated with biological systems.

References

[1] Ham, D., Park, H., Hwang, S. & Kim, K. Neuromorphic electronics based on copying and pasting the brain. Nat. Electron. **4**, 635–644 (2021).
[2] Zhang, W. et al. Neuro-inspired computing chips. Nat. Electron. **3**, 371–382 (2020).
[3] Gkoupidenis, P., Schaefer, N., Garlan, B. & Malliaras, G. G. Neuromorphic functions in PEDOT:PSS organic electrochemical transistors. Adv. Mater. **27**, 7176–7180 (2015).
[4] van de Burgt, Y. et al. A non-volatile organic electrochemical device as a low-voltage artificial synapse for neuromorphic computing. Nat. Mater. **16**, 414–418 (2017).
[5] Gkoupidenis, P., Koutsouras, D. A. & Malliaras, G. G. Neuromorphic device architectures with global connectivity through electrolyte gating. Nat. Commun. **8**, 15448 (2017).
[6] Sarka, T. et al. An organic artificial spiking neuron for in situ neuromorphic sensing and biointerfacing. Nat. Electron. **5**, 774-783 (2022).

O 1.3

Print the Brain: Neuromorphic 3D-Circuits Based on Printed Organic Memristors

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Memristors as resistive switches are not only very interesting as components for neuromorphic circuit concepts; their simpler layer structure compared to transistors also lends itself directly to printing. However, in order to realize neuromorphic circuits, a three-dimensional structure is necessary. This can be achieved by a massive multi-stack design, which enables roll-to-roll production.

In this presentation, a promising printable device and material concept for filament-type memristors will be introduced [1] and the processability will be investigated. The performance achievable today will be discussed.

Furthermore, solutions for the fabrication of massive multistack 3D circuits using memristors are presented. The mechanical properties and boundary conditions for the design of the memristors and conceivable interconnections are analyzed for the proposed roll-to-roll fabrication.

References

[1] Strutwolf, J.; Chen Y.; Ullrich, J.; Hübler, Arved C.: Memristive devices based on mass printed organic resistive switching layers. Appl. Phys. A 127, 709 (2021)

O 1.4

Direct Recording of Action Potentials of Cardiomyocytes Through Printed Electrolyte-Gated Field-Effect Transistors

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Minimally invasive recording of intracellular action potentials in electrogenic cells is in high demand. Most of present electronic probing tools are either invasive or require complex manufacturing processes. With the aim of enabling a cost-effective, non-invasive probing platform based on devices that can be easily fabricated and processed from solution with large-area printing techniques, we propose planar Electrolyte Gated Field-Effect Transistors (EGFETs) based on solution-processed based carbon-based material. Remarkably, despite the planar geometry of the device, we could demonstrate the spontaneous recording of intracellular action potentials from a monolayer of human induced pluripotent stem cells derived Cardiomyocytes. The effect of drugs on the frequency and duration of the Action Potential was investigated. The simplicity of the device combined with the high signal to noise ratio opens up new opportunities for low-cost, reliable, and flexible biosensors and arrays for high quality parallel recording of cellular action potentials.

O 1.5

Cell mechanotransduction driven by bio-organic optoelectronic devices

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Biophysical cues, especially mechanosensation, play a fundamental role throughout life, starting from early embryonic development over function and interplay of cells and tissues in the adult body up to regeneration processes. Tissue regeneration, which includes phenomena like cell division, differentiation, migration and expulsion is triggered by extracellular mechanical cues [1,2,3]. The body's capability to regenerate decreases with age and therefore impacts our life in sometimes detrimental aspects. Currently available tools to modulate or control mechanosensation often lack features necessary for *in vitro* and *in vivo* applications, in terms of efficiency, reliability, reversibility and spatial sensitivity.

Here, we show a novel approach to control mechanosensitive ion channels, through exogenous organic semiconductors. Materials in this class are fully biocompatible, thus offering the perspective for in vivo application, they can be easily processed in several forms, such as thin films, microstructured devices or nanoparticles. Most importantly, they are characterized by distinctive opto-electrical properties, providing excellent visible light responsivity, as well as electron and ion conductivity.

In this work we originally explore the opportunity to use organic semiconductors, and in particular conjugated polymers, to remotely control the activation of mechano-sensitive ion channels, in a reliable, touchless and effective manner. We critically discuss results obtained with different tools, including polymer thin films and microstructured devices.

Our results may contribute to develop innovative smart materials for tissue regeneration driven by optical and electrical cues.

References

[1] M. Bielfeldt, H. Rebl, et al.; Biomedical Materials and Devices, (2022)
[2] S.A. Gudipaty, J. Lindblom et al.; Nature 543 (7643):118-121 (2017)
[3] M. Aragona, A. Sifrim et al. Nature 584 (7820):268-273 (2020)

O 1.6

Membrane Targeted Azobenzene Drives Optical Modulation of Bacterial Membrane Potential

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The possibility to control living matter with exogenous stimuli can have tremendous impact on synthetic biology, medicine and materials science, among others. For instance achieving control over cells behaviour remains a challenge at the interface between living and non-living matter,[1] and would enable the development of new bio-mimetic and bio-enabled materials able to perform tasks.[2] Within this context, bacteria have arisen as "active and actively-controllable materials", exhibiting neuro-like behaviour, extended bioelectric signalling[3,4] and tunable assembly properties.[5] In the last decade, it has been observed that the regulatory element of such an active behaviour is the electrical potential across the membrane, which governs bacteria electrophysiology, metabolisms and bioenergetics.[6] Light can be a powerful tool in these regards, as one can control the membrane potential and, thus, cell function and behaviour remotely and with relatively high spatiotemporal precision.

Here, I will show that a membrane-targeted azobenzene can be used to photo-modulate precisely the membrane potential in cells of the Gram-positive bacterium *Bacillus subtilis*. We found that upon exposure to blue- green light, the isomerization reaction in the bacteria membrane induces hyperpolarisation of the potential ($\Delta V = 20$ mV), within a bio-mimetic mechanism reproducing the initial fate of retinal. Apart from being promising results in the view to photocontrol bacterial motion and assembly behavior in consortia, this approach also highlights the role of previously uncharacterized ion channels in bacteria electrophysiology.[7]

References

[1] C. Xu, N. Martin, M. Li, S. Mann, *Nature* **2022**, *609*, 1029.

[2] F. Zhang, Z. Li, Y. Duan, A. Abbas, R. Mundaca-Uribe, L. Yin, H. Luan, W. Gao, R. H. Fang, L. Zhang, J. Wang, *Sci. Robot.* **2022**, *7*, 1.

[3] J. M. Kralj, D. R. Hochbaum, A. D. Douglass, A. E. Cohen, *Science (80-.).* **2011**, *333*, 345.

[4] A. Prindle, J. Liu, M. Asally, S. Ly, J. Garcia-Ojalvo, G. M. Süel, *Nature* **2015**, *527*, 59.

[5] V. E. Johansen, L. Catón, R. Hamidjaja, E. Oosterink, B. D. Wilts, T. S. Rasmussen, M. M. Sherlock, C. J. Ingham, S. Vignolini, *Proc. Natl. Acad. Sci. U. S. A.* **2018**, *115*, 2652.

[6] J. M. Benarroch, M. Asally, *Trends Microbiol.* **2020**, *28*, 304.

[7] T. C. de Souza-guerreiro, G. Bondelli, I. Grobas, S. Donini, V. Sesti, C. Bertarelli, G. Lanzani, M. Asally, G. M. Paternò, *Adv. Sci. 2023, 2205007*

O 1.7

Chiral emission from halide perovskite semiconductors

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Spin polarized light-emitting diodes (Spin-LEDs) convert spin information to helicity of the emitted photon, which allows long-distance communication and exchange of non-classical information. In a conventional spin-LED, spin-polarized carriers have been achieved through the ferromagnetic electrode or external magnetic field, which requires dedicated control of film growth of spin-injector layer and emitting layer to polarize and maintain spin polarization as well as strict device operation conditions (e.g. low temperatures). Moreover, limitations of spin injection efficiency in the presence of injection/emitter interface remains unsolved. Here, we report a spin- -LED based on low-dimensional chiral perovskite semiconductors, within which spin selection occurs. By performing inverse spin Hall effect measurements, we demonstrate that the spin polarized carriers are accumulated due to the chiral induced spin selectivity (CISS) effect. Strong circularly polarized electroluminescence (CP-EL) is achieved through efficient spin transfer in low-dimensional perovskites, as evidenced by circularly polarized pump-probe transient absorption spectroscopy. We have been able to simultaneously obtain a large EL polarization of ± 6 % and high LED performance at room temperature, enabling future applications for spin-lasers and quantum communications.

O 1.8

Mastering morphology of non-fullerene acceptors towards long-term stable organic solar cells

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As an important representative of the emerging photovoltaic technology, organic photovoltaics (OPV) can achieve excellent device performance and low-cost, continuous production and processing through solution printing technology, and are expected to make outstanding contributions to solar-driven multifunctional applications. In order to realize the industrialization and commercial application of OPV technology, research teams around world have made a lot of efforts. In the past few years, through the synthesis of new materials, optimization of thin film micro-morphology, and development of advanced processing technologies, the power conversion efficiency of OPV devices has been continuously improved. However, the stability of OPV devices is a key issue that still restricts the industrialization of OPV technology. In this contribution, I will discuss our recent progress on the stability of OPV devices, and propose some effective solutions to solving the instability problems, including the development of oligomer acceptors,[1] the use of single-component OPV devices,[2] and the use of multiple component strategy,[3,4] etc., so as to further promote the new generation of OPV devices to achieve excellent performance and stability.

References

[1] Y. Liang, D. Zhang, Z. Wu, T. Jia, L. Lüer, H. Tang, J. Zhang, J. Jia, K. Zhang, C. J. Brabec, N. Li, F. Huang, "Organic solar cells using oligomer acceptors for improved stability and efficiency," Nature Energy **7**, 1180-1190 (2022).

[2] Y. He, N. Li, T. Heumüller, J. Wortmann, B. Hanisch, A. Aubele, S. Lucas, G. Feng, X. Jiang, W. Li, P. Bäuerle, C. J. Brabec, "Industrial viability of single-component organic solar cells," Joule **6**, 1160-1171 (2022).

[3] K. An, W. Zhong, F. Peng, W. Deng, Y. Shang, H. Quan, H. Qiu, H. Wu, N. Li, F. Huang, L. Ying, "Mastering microstructure morphology of non-fullerene acceptors towards long-term stable organic solar cells," Nature Communications **14**, 2688 (2023).

[4] C. Liu, L. Lüer, V. M. Le Corre, K. Forberich, P. Weitz, T. Heumüller, X. Du, J. Wortmann, J. Zhang, J. Wagner, L. Ying, J. Hauch, N. Li, C. J. Brabec, "Understanding causalities in organic photovoltaics device degradation in a machine-learning-driven high-throughput platform," Advanced Materials 2300259 (2023).

O 1.9

Organic Electronic Materials via Cascade Synthetic Approach based on One Pot DHA-Perkin Annulations

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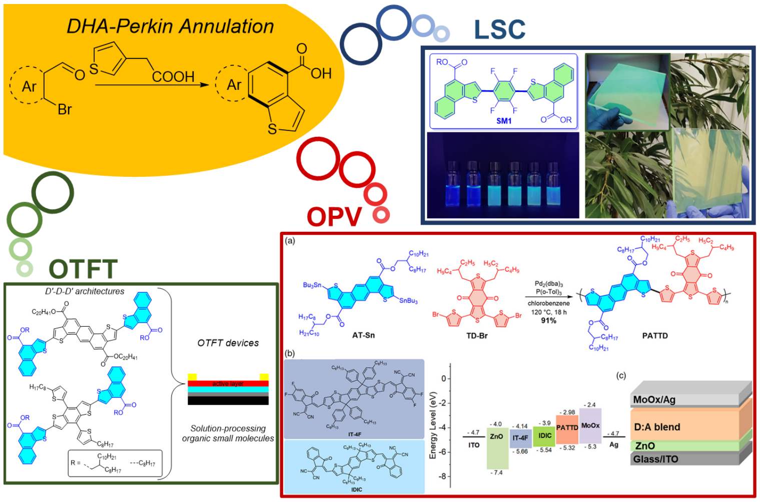
Organic electronics offers well-known advantages such as flexibility, low cost, and easy processability using simple solutions processing methods. Organic electronics technologies utilize π-extended organic compounds and polymers, typically obtained with linear type multi-step synthesis. However, it is worth noting that this approach led to compounds and polymers have traditionally been obtained through complex, multi-step synthesis approaches, limiting scalability for industrial applications. Sustainability and scalability of the synthetic process plays a fundamental role for definitive consecration of the organic electronic technologies, and generally it depends on: (a) the number of synthetic steps; (b) the cost of the materials; (c) yields; (d) the number of steps of purification that require column chromatography.
In this contribute we will report our recent developments on the use of one-pot cascade direct (hetero)arylation (DHA) and intramolecular Perkin condensation protocol for the annulation and π–extension of compounds and polymers incorporated in OPV, LSC and OTFT devices.[1-4] The application of such protocol has been used with success for the synthesis of thienoacene scaffolds such as naphthothiophenes (NTs), benzodithiophenes (BDTs) and anthradithiophenes (ADTs) in a single and double annulation fashion. ADT and BDT derivatives were incorporated into polymers and the properties of bulk-heterojunction solar cells will be presented.[1,2] Novel NT-based small molecules with aggregation-induced emission (AIE) or conducting behaviours will be presented, and their properties in LSC and OTFT devices will be discussed.[3,4]



References

[1] G. Bianchi, C. Carbonera, L. Ciammaruchi,* N. Camaioni, N. Negarville, F. Tinti,* G. Forti, A. Nitti,* D. Pasini, A. Facchetti, R. M. Pankow, T. J. Marks, R. Po, *Sol. RRL* **2022**, *6*, 2200643.
[2] M. Penconi, G. Bianchi, A. Nitti, A. Savoini, C. Carbonera, D. Pasini, R. Po, S. Luzzati. *Adv. Energy Sustainability Res.* **2021**, *2*, 2100069.
[3] A. Nitti, F. Corsini, E. Tatsi, G. Mattioli, C. Botta, D. Pasini,* G. Griffini,* *Adv. Optical Mater.* **2021**, *9*, 21001.
[4] A. Nitti, G. Forti, G. Bianchi, C. Botta, F. Tinti, M. Gazzano, N. Camaioni, R. Po, D. Pasini,* *J. Mater. Chem. C* **2021**, *9*, 9302-9308.

O 1.10

Metal-TetraPhenyl-Porphyrins Adsorption on Atom-Thick and Bulk Magnetic Oxides

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Metal tetraphenyl porphyrins (M-TPP) can host different metal ions within their tetra-pyrrole ring, providing exceptional flexibility in the molecular properties and functions. Molecular layers of M-TPP typically self-assemble on surfaces forming square-like superlattices of planar molecules with a high degree of structural order. That makes them an ideal benchmark for the study of their properties by surface science techniques and facilitates applications where well-defined hybrid interfaces are requested. Additionally, these ordered layers can pave the ground to the subsequent growth of 3D molecular architectures. Among supporting surfaces, oxides and oxidized layers raise interest because of their intrinsic properties (e.g., as antiferromagnetic substrates for organic spintronics [1]), or as protective layers.

We have combined experimental techniques and ab initio methods based on density functional theory (DFT) to investigate Co-, Ni-, Zn-, and VO-TPP molecules adsorbed on an atom-thick oxide [namely Fe(001)-p(1x1)O] where the oxide layer is able to preserve the characteristic features of quasi-free molecules as we evidence by UV-photoemission/inverse photoemission spectroscopy and calculations.[2] Adsorption structures are characterized by well ordered 5x5 superlattices that can attain different orientations depending on the central atom, despite a moderately-dependent computed energetics points to a subtle influence.[3] DFT analysis also points to a dominant antiferromagnetic coupling between the molecular spin and the substrate one. VO-TPP, which further offer an additional degree of freedom through the V=O bond orientation, also form square ordered superstructures with both upwards and downwards cases possible.[4]

The interaction of a selected cases (Co-TPP) at the surface of antiferromagnetic NiO substrate is then studied as a prototypical case for perspective antiferromagnetic spintronics applications.[1] Calculations allow us to identify the adsorption site for Co atop Ni, facilitating magnetic coupling between the molecule and the surface despite the absence of a net substrate magnetization.

References

[1] SINFONIA FET project, grant n. 964396 - www.sinfonia-fet.eu

[2] A. Calloni et al, "Cobalt atoms drive the anchoring of Co-TPP molecules to the oxygen-passivated Fe(0 0 1) surface", Applied Surface Science **505**, 144213 (2020).

[3] G. Fratesi et al, "Nontrivial central-atom dependence in the adsorption of M-TPP molecules (M = Co, Ni, Zn) on Fe(001)- p (1 × 1) O", Applied Surface Science **530**, 147085 (2020).

[4] G. Albani et al, "Ordered assembly of non-planar vanadyl-tetraphenylporphyrins on ultra-thin iron oxide", PCCP Phys. Chem. Chem. Phys., **24**, 17077 (2022).

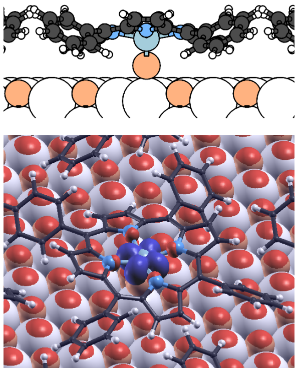

Figure 1. *Structural model of VO-TPP adsorbed on Fe(001)-p1x1O (top) and corresponding spin density (red/blue=spin majority/minority).*

O 1.11

Paradigm Shift in Iridium Emitters Structure: Single Active Ligand in Heteroleptic Complexes for NIR Phosphorescent OLEDs

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Near-infrared (NIR) phosphorescent organic light-emitting diodes (PhOLEDs) are gaining increasing attention due to their potential applications in bio-imaging, night-vision displays, communication and security systems.[1] In this field, Ir(III) complexes, the emitters of choice in commercial visible-light OLEDs, represent the most promising candidates given their exceptional versatility and stability. When the chemical structure of a Ir(III) complex is engineered to push the emission towards the NIR, the preservation of good phosphorescence quantum efficiency and ease of material processing is highly challenging.

In this communication, we present our strategy for the chemical design of the C^N ligand in Ir(III) complexes to lower the emission energy through the expansion of the π-system and the introduction of substituent with different electronic effects without hampering phosphorescence efficiency. A family of novel Ir(III) complexes is synthesized, investigated by optical spectroscopy, electrochemistry and theoretical calculations and finally employed in PhOLEDs, highlighting the structure-property-performance relationships. Moreover, we propose a novel approach for the construction of the complex by employing only one NIR-active C^N ligand and two 'dark' ligands, with important advantages in terms of synthesis and material processing.[2] We demonstrate that the presence of a single C^N ligand is sufficient to enable NIR phosphorescence of quantum efficiency comparable to the homoleptic and bis-heteroleptic complexes and superior efficiency in fully-evaporated OLEDs.

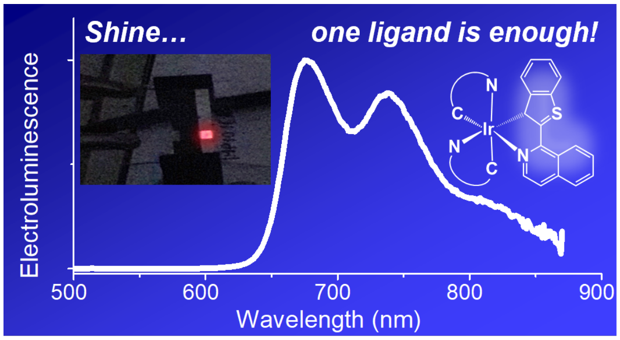

Figure 1. Near-Infrared electroluminescence in OLEDs based on heteroleptic Ir(III) complex bearing a single emitting ligand.

References

[1] A. Zampetti, A. Minotto, and F. Cacialli, "Near-Infrared (NIR) Organic Light-Emitting Diodes (OLEDs): Challenges and Opportunities", Adv. Funct. Mater. **29**, 1–22 (2019).

[2] M. Penconi, A. Babu Kajjam, M.-C. Jung, M. Cazzaniga, C. Baldoli, D. Ceresoli, M. E. Thompson, A. Bossi, "Advancing Near-Infrared Phosphorescence with Heteroleptic Iridium Complexes Bearing a Single Emitting Ligand: Properties and Organic Light-Emitting Diode Applications", Chem. Mater. **34**, 574−583 (2022).

O 1.12

Organic Photodetectors and their tolerance to impurities

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Poly[[6,7-difluoro[(2-hexyldecyl)oxy]-5,8-quinoxalinediyl]-2,5-thiophenediyl]] (PTQ10) has become one of the most famous polymers in the field of organic photovoltaics, yet it has only been scarcely used in organic photodetectors [1-3]. It is a relatively low-cost donor polymer, obtained in few steps, including a Stille coupling polymerization, starting from cheap precursors with an overall yield > 85% [4]. While some studies exist for OPVs [5, 6], the effect of residual catalyst on the performances of OPDs has, to date, not been investigated.

We report here the fabrication and characterization of OPDs integrating the PTQ10:ITIC-F system into an inverted structure Glass/ITO/ZnO/PEIE/active layer/MoOx/Ag, for the detection of visible light. Following the optimization of the deposition process we achieved state-of-the-art devices with responsivity as high as 0.5 A/W. The impact of the introduction of various synthesis-related impurities is then investigated. Results show that some impurities (e.g. both the catalyst and its PPh3 ligand) are critical, at a relatively low concentration of few hundreds of ppm (or ppm eq) of Pd, evidencing the need for polymers to be highly purified for OPD applications.

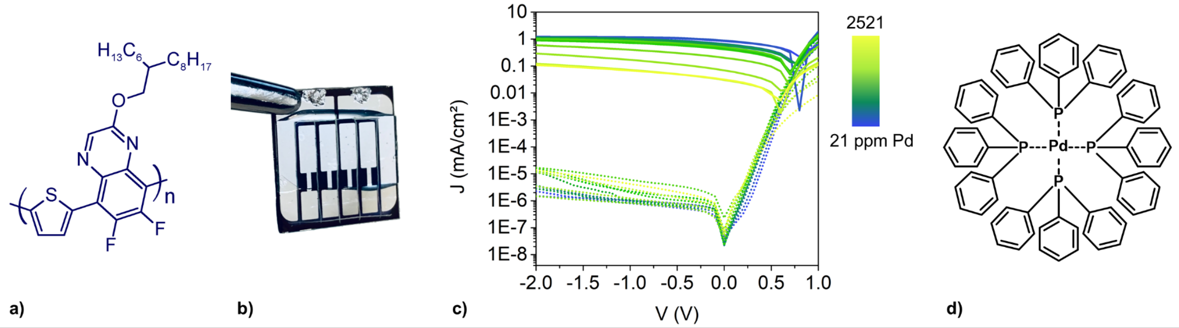

Figure 1. a) chemical structure of PTQ10, b) picture of an encapsulated sample with 4 central OPDs, c) J-V characteristics in the dark (dotted lines) and under 25 W/m² irradiance at 528 nm (solid lines) for different concentrations of $Pd(PPh_3)_4$ impurity (in ppm of Pd) and d) chemical structure of $Pd(PPh_3)_4$.

References

[1] H. Bristow, P. Jacoutot, A. D. Scaccabarozzi, M. Babics, M. Moser, A. Wadsworth, T. D. Anthopoulos, A. Bakulin, I. McCulloch, N. Gasparini, ACS Appl. Mater. Interfaces 2020, 12, 48836.
[2] T. Zhang, M. Moser, A. D. Scaccabarozzi, H. Bristow, P. Jacoutot, A. Wadsworth, T. D. Anthopoulos, I. McCulloch, N. Gasparini, J. Phys. Mater. 2021, 4, 045001.
[3] P. Kafourou, Z. Qiao, M. Tóth, F. Aniés, F. Eisner, N. Gasparini, M. Heeney, ACS Appl. Mater. Interfaces 2022, acsami.2c10197.
[4] C. Sun, F. Pan, H. Bin, J. Zhang, L. Xue, B. Qiu, Z. Wei, Z.-G. Zhang, Y. Li, Nat Commun 2018, 9, 743.
[5] C. Bracher, H. Yi, N. W. Scarratt, R. Masters, A. J. Pearson, C. Rodenburg, A. Iraqi, D. G. Lidzey, Organic Electronics 2015, 27, 266.
[6] N. Schopp, V. V. Brus, J. Lee, A. Dixon, A. Karki, T. Liu, Z. Peng, K. R. Graham, H. Ade, G. C. Bazan, T. Nguyen, Adv. Funct. Mater. 2021, 31, 2009363.

O 1.13

Excitation “memory” accelerates transient electroluminescent response of quantum-dot light-emitting diodes

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Quantum-dot light-emitting diodes (QLEDs), a class of solution-processed EL devices based on organic-inorganic hybrid structures, show great potential in next-generation optoelectronics. Understanding their transient response dynamics is essential for developing high-speed devices for EL display, light communications [1] and potentially electrically-pumped lasing [2].

Here, we report that the transient responses of the QLED can be accelerated by the “memory” of its excitation history, distinguishing QLEDs from conventional inorganic LEDs (Fig. 1a). We elucidate that this transient behavior originates from the interplay between transient EL processes and deep-level fast traps in the organic hole-transport layer, which generates a new fast-response EL channel that occurs in high-frequency operations. Finally, we harness this transient response pathway on a micro-QLED, demonstrating high-speed modulations up to 100 MHz at a moderate excitation level of ~200 mA cm^{-2} (Fig. 1b).

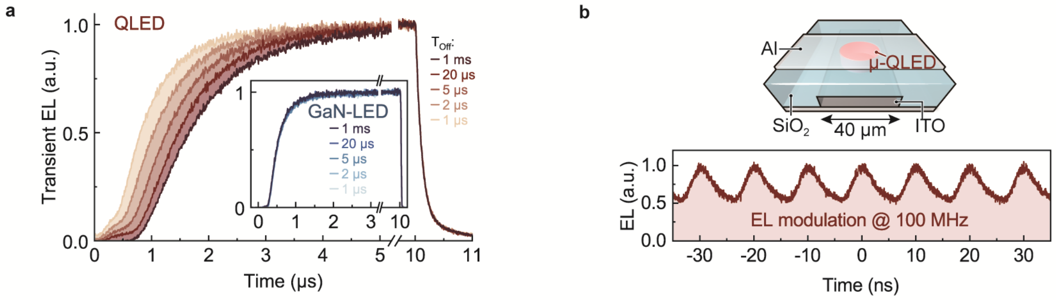

Fig. 1 Excitation-memory accelerated transient response of QLED (**a**) enables fast response in high-speed operations (**b**).

This work highlights a universal transient EL behavior dominated by trap-related processes in the organic charge-transport materials, which is found to be generally exists in solution-processed LEDs employing organic hole-transport materials, including perovskite LEDs and polymer LEDs. We except that the excitation-memory induced fast-response dynamics could facilitate the realization of solution-processed, low-power, and fast-response EL devices.

References

[1] Ren, A., et al., “Emerging light-emitting diodes for next-generation data communications”. Nat. Electron. **4,** 559-572 (2021).

[2] Ahn, N., et al., “Electrically driven amplified spontaneous emission from colloidal quantum dots”. Nature, **617,** 79-85 (2023).

O 1.14

Chemical insights into perovskite inks behavior and their implications in photovoltaic devices

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Metal halide perovskite (MHP) semiconductors are excellent candidates for contemporary optoelectronics innovation, particularly for photovoltaics.[1] The advantages of this class of materials derive from their hybrid nature, allowing for straightforward fabrication processes, and from their unique optoelectronic properties. A typical 3D organic-inorganic perovskite has a chemical formula of ABX3, where A is an organic cation (such as MA [methylammonium] or FA [formamidinium]), B is a metal cation (such as Pb2+), and X is a halogen anion (such as I or Br).[2] However, recent advances have also explored more complex compositions embedding diverse cations/anions.[3] These materials are prepared by simple and straightforward solution processing, the material precursors dissolved in a solvent undergoes self-assembly into a perovskite structure during spin-coating onto a substrate under mild thermal annealing. As the technology continues to mature, this still is a key advantage, allowing for affordable and scalable processing. Understanding perovskite ink properties is therefore a fundamental requirement towards industrialization, with special regards to their evolution over time.

It has been demonstrated that even for the simplest system, the precursor solution is a complex – and dynamic – dispersion which contains not only solvated ions but also lead halide complexes, colloids and aggregates of different natures and dimensions. In these complex dispersions, multiple chemical species are present and can interact – or react – between each other or with the solvent.

We have proved the existence of a reactivity between two of the perovskite components – methylammonium and formamidinium – in the precursors solutions, that leads to ink variations over time, which in turn means variation in the final polycrystalline material properties. In fact, the characteristics of precursor solution eventually dictate the optoelectronic quality of resulting perovskite films that proceed with the solution aging and determine undesirable decrease of solar cells performances. We have studied different parameters that affects such reactions kinetics and proposed solutions to overcome these issues.[4]

Starting from the known reactivity of the chemical species present in ink solutions, we outline the directions towards which future research efforts should be directed.[5]

References:

[1] Jeong, J., Kim, M., Seo, J., Lu, H., Ahlawat, P., Mishra, A., Yang, Y., Hope, M.A., Eickemeyer, F.T., Kim, M., et al. (2021). Pseudo-halide anion engineering for α-FAPbI3 perovskite solar cells. Nature 592, 381–385.
[2] Snaith, H.J. (2013). Perovskites: The emergence of a new era for low-cost, high-efficiency solar cells. Journal of Physical Chemistry Letters 4, 3623–3630.
[3] McMeekin, D.P., Sadoughi, G., Rehman, W., Eperon, G.E., Saliba, M., Hörantner, M.T., Haghighirad, A., Sakai, N., Korte, L., Rech, B., et al. (2016). A mixed-cation lead mixed-halide perovskite absorber for tandem solar cells. Science 351, 151–155.
[4] Valenzano, V., Cesari, A., Balzano, F., Milella, A., Fracassi, F., Listorti, A., Gigli, G., Rizzo, A., Uccello-Barretta, G., and Colella, S. (2021). Methylammonium-formamidinium reactivity in aged organometal halide perovskite inks. Cell Reports Physical Science 2, 100432.
[5] Rizzo A., Listorti A., Colella S. (2022). Chemical insights into perovskite ink stability. Chem, 8, 1, 31-45.

O 1.15

Tuning the magnetic properties of antiferromagnetic oxides via adsorption of organic molecules: pentacene on NiO(001)

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Organically functionalized solid surfaces are a very active field of research, thanks to the tunability of molecular electronic properties, which can, in turn, modify the properties of the substrate. In "spinterfaces" the molecular overlayer can tune the spin polarization of the magnetic substrate surface, with potential applications in spintronics. We perform first-principles studies on the structural, electronic, magnetic and optical properties of interfaces between organic molecules and antiferromagnetic substrates, i.e. both bulk and ultrathin transition metal oxides, within the joint computational/experimental SINFONIA project ("Selectively activated INFOrmation technology by hybrid Organic Interfaces") [1]. The project is aimed at exploring the possibility of developing devices that enable the conversion of an optical stimulus applied to an organic molecule adsorbed on a solid surface to a propagating magnetic perturbation (spin wave) within the substrate and backwards with extreme spatial and temporal resolutions. Here I will report on a monolayer of pentacene adsorbed on the nickel oxide (001) surface.

In our density functional theory (DFT) calculations with Hubbard correction (DFT+U), we considered surface unit cells and molecule orientations based on low-energy electron diffraction (LEED), angle-resolved photoemission (ARPES) and scanning tunneling (STM) measurements. The Ni-Ni bridge adsorption sites are found to be energetically favored. On the most stable pentacene/NiO(001) adsorption configurations, we compute electronic and magnetic properties. The effects on surface and molecule magnetization for molecule adsorption on the (001) surface of bulk NiO are mild and depend on the orientation of the molecule with respect to the magnetically anisotropic surface (Fig. 1). Preliminary results suggest instead much larger effects for molecule adsorption on ultrathin NiO. We also investigate the optical properties of the adsorbed system, focusing on spectral features due to molecule adsorption.

References

[1] www.sinfonia-fet.eu

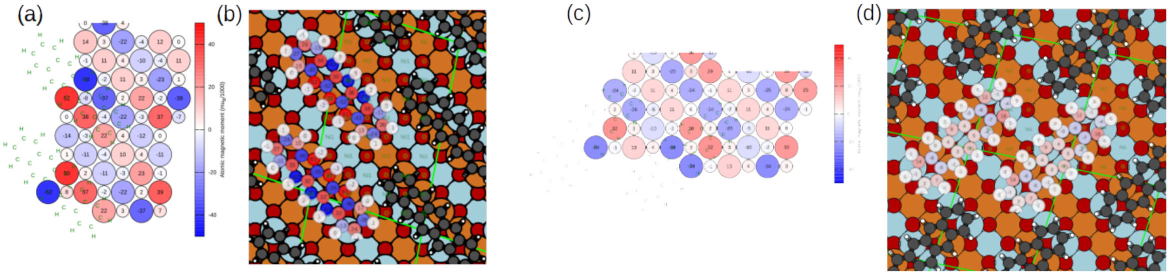

Fig. 1: Most stable pentacene/NiO(001) configurations: modifications to the magnetic moments of the surface (a,c) and magnetic moments induced on the molecule (b,d) upon adsorption. Color scale from -0.05 μ_B (blue) to 0.05 μ_B (red).

O 2.1

Copper Phthalocyanine Based Electrochemical Transistors for Future Edible Electronics

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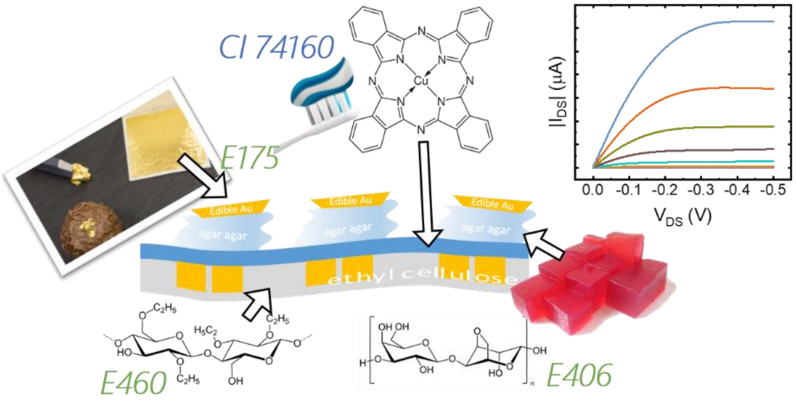

Edible Electronics [1] is an emerging field targeting devices that can be safely ingested and that, after functioning, can be digested, as food. Relevant applications can be envisioned both in the healthcare and the food supply chain sectors, among all: non-invasive monitoring of the gastrointestinal tract, smart and controlled drug release systems, smart tags for safe and direct food tagging and real-time food quality check. One of the main challenges of this research field is represented by the identification of well performing non-toxic semiconductors, to be integrated into **low voltage driven (<1V) edible transistors** architecture. In this regard, Copper Phthalocyanine (CuPc), also known as C.I. Pigment Blue 15 (CI 74160) is a well-established, biocompatible pigment. While insoluble in most solvents, vacuum deposited CuPc films have been efficiently employed as semiconductor both in solar cells and organic field effect transistors. Nevertheless, its commercial use is mostly associated to its optical and chemical attributes, and it should come as no surprise that it is widely used as teeth whitener into commercially available and popular toothpaste formulations. We recently observed that t**he average amount of CuPc already safely ingested during daily teeth brushing exceeds by several orders of magnitude the estimated amount needed into our electronic systems**, this making CuPc a strong candidate as the semiconductor of edible devices. Of course, its employment requires the individuation of effective, scalable processing strategies, on the one hand compatible with edible substrates, like polysaccharides, which are usually highly soluble and thermally instable; on the other hand forming film nanostructures that efficiently support charge transport. Here we report on the possibility to integrate CuPc films with long-range crystallinity and tunable morphology into fully edible devices, based on a Floating Film Transfer Method. **We show that an unconventional solution process, based on reversible molecular protonation, can be used, notably resulting in films with effective ion permeation from electrolytic solutions.** Following this strategy, stable electrochemical transistor with hydrogel-based architecture, entirely composed of edible materials, is finally demonstrated. The herein obtained **on/off ratios overcoming 10^3 and trans-conductance up to 0.6 mS (≈7 μS/mm)** qualify our devices both as a suitable platform for sensing and bio-sensing and as active components of low voltage edible integrated circuits.

[1] AS Sharova, F Melloni, G Lanzani, CJ Bettinger, M Caironi, “Edible electronics: The vision and the challenge” Advanced Materials Technologies 6 (2), 200075

O 2.2

Permeable electronic skins for health monitoring

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One limitation of commercialized wearables, such as smartwatches and bands, is that they cannot form conformable contact with human skin due to their rigid form factor, thereby limiting their monitoring capabilities. Soft bioelectronics, on the other hand, are touted as an ideal platform for personalized health care owing to unique characteristics, such as thinness, lightweight, good biocompatibility, excellent mechanical robustness, and great skin conformability. Permeable skin-mountable electronics that are capable of long-term applications have emerged as promising tools for early disease prevention, screening, diagnosis, and treatment[1,2]. Dr. Wang's research interests mainly focus on the development of wearable electronics for biomedical health monitoring, including stretchable conductors, sensors, and soft energy devices. In today's talk, she will introduce high-performance skin bioelectronics developed by ultrasoft nanomesh systems, which can realize the accurate measurement of minus skin deformations and finger touch without disturbing natural skin motions and sensations, as well as long-term applications for health monitoring[3-5].

References

[1] A. Miyamoto, S. Lee, N.F. Cooray, S. Lee, M. Mori, N. Matsuhisa, H. Jin, L. Yoda, T. Yokota, A. Itoh, M. Sekino, T. Someya, "Inflammation-free, gas-permeable, lightweight, stretchable on-skin electronics with nanomeshes," Nat. Nanotechnol. **12**, 907-913 (2017).

[2] J. Yang, Z. Zhang, P. Zhou, Y. Zhang, Y. Liu, Y. Xu, Y. Gu, S. Qin, H. Haick, Y. Wang, "Toward a new generation of permeable skin electronics," Nanoscale **15**, 3051-3078 (2023).

[3] Y. Wang, S. Lee, H. Wang, Z. Jiang, Y. Jimbo, C. Wang, B. Wang, J.J. Kim, M. Koizumi, T. Yokota, T. Someya, "Robust, self-adhesive, reinforced polymeric nanofilms enabling gas-permeable dry electrodes for long-term application," PNAS **118**, e2111904118 (2021).

[4] Y. Wang, S. Lee, T. Yokota, H. Wang, Z. Jiang, J. Wang, M. Koizumi, T. Someya, "A durable nanomesh on-skin strain gauge for natural skin motion monitoring with minimum mechanical constraints," Sci. Adv. **6,** eabb7043 (2020).

[5] S. Lee, S. Franklin, F.A. Hassani, T. Yokota, M.O.G. Nayeem, Y. Wang, R. Leib, G. Cheng, D.W. Franklin, T. Someya, "Nanomesh pressure sensor for monitoring finger manipulation without sensory interference," Science **370**, 966-970 (2020).

Profile:

Dr. Yan Wang is currently an Associate Professor at Guangdong Technion. She received her Ph.D. degree majoring in Chemical Engineering from Monash University in 2018 and completed her postdoc training at the Department of Electrical and Electronic Engineering, at the University of Tokyo, in 2021. In soft electronics field, Dr. Yan Wang has published over 40 scientific articles in flagship journals like Science, Nature Electronics, Science Advances, PNAS, Chemical Society Reviews, ACS Nano, etc., 21 with IF > 10, h-index of 25, 3 ESI highly cited papers, granted 1 Australia patent and applied for 2 US patents, and won several scientific awards, such as 2018 Outstanding Self-financed Students Abroad. Her research works were featured by renowned CNN, Science, major Australian media such as Herald Sun, and Japanese media such as Nikkan Kogyo Shimbun. At Guangdong Technion, her group mainly focuses on materials development and the practical implementation of soft wearables in real-life situations towards ambulatory health care and the Internet of Things.

O 2.3

2D/3D-Printed Flexible Organic Thermoelectrics for Low-Scale Energy Harvesting

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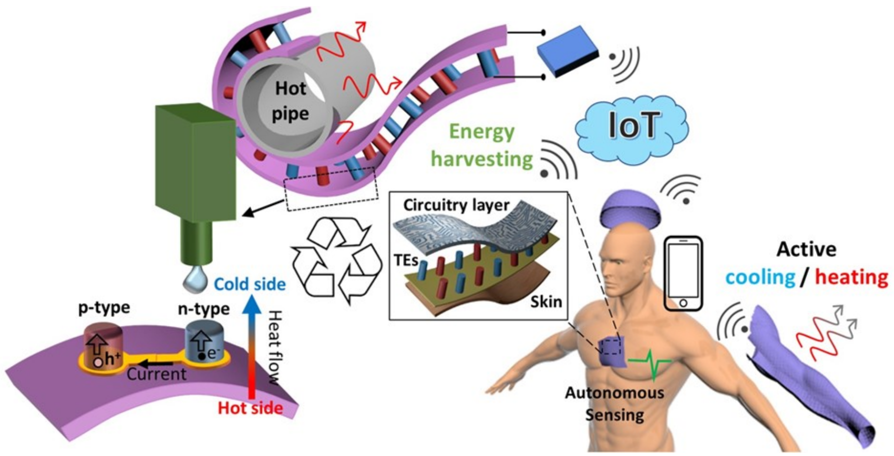

Distributed electronics are gaining traction for application in wearables and the internet of things (IoT). In both cases, the increasing complexity of the systems comes along an acute need for energy. Batteries struggle to satisfy this need, either because they are too bulky to be seamlessly integrated on thin wearable electronics, or because their replacement is unfeasible for the numerous and highly-distributed nodes of the IoT. Rechargeable (thin-film) batteries represent an opportunity, but they must be coupled with an energy harvester that can provide renewable energy. In those scenarios, thermoelectric (TE) materials, which can convert directly waste heat into electrical power, hold a great promise. Conveniently, it has been suggested that TEs are more efficient than other thermal engines for low power applications like wearables and the IoT.[1] However, the widespread of TE generators (TEG) is hampered by their expensive fabrication process; the use of critical elements such as Bi, Sb; and their limited form factor (rigid, flat and small).[2] The ubiquity of the IoT nodes and the particular form factor of wearable devices (stretchable and large-area) call for a new technology that strongly relies on clean and abundant materials like polymers, and on new fabrication techniques allowing their integration in devices with unconventional form factors.

In my research group, we are working towards the development of high-performing organic TE materials, which can be directly printed over large areas on flexible/stretchable substrates. Printing techniques are not only potentially cheap and suitable for conducting polymers and soft substrates, but offer also a process versatility that enables material morphology tuning and original device architectures. Indeed, the bulk nature of TEs encouraged us to go beyond the traditional 2D printing techniques and to exploit the third dimension via 3D printing. We aim at performing organic TE materials integrated in devices that can be easily mounted on the skin to power wearables using the heat emitted by the human body, or to tightly conform to hot curved surfaces, like hot pipes or engines, to power IoT nodes. If successful, this line of research will holistically tackle the three main bottlenecks of TEG mentioned above, paving the way to the broad implementation of TEs in wearables and other low-power energy harvesting applications.

References

[1] C. B. Vining, “An inconvenient truth about thermoelectrics,” *Nat. Mater.*, vol. 8, no. 2, pp. 83–85, Feb. 2009, doi: 10.1038/nmat2361.

[2] F. Molina-Lopez, “Emerging Thermoelectric Generators Based on Printed and Flexible Electronics Technology,” in *2020 IEEE Sensors*, Oct. 2020, pp. 1–4. doi: 10.1109/SENSORS47125.2020.9278922.

O 2.4

Ambipolar Blend-based Organic Mixed Ionic-Electronic Conductors

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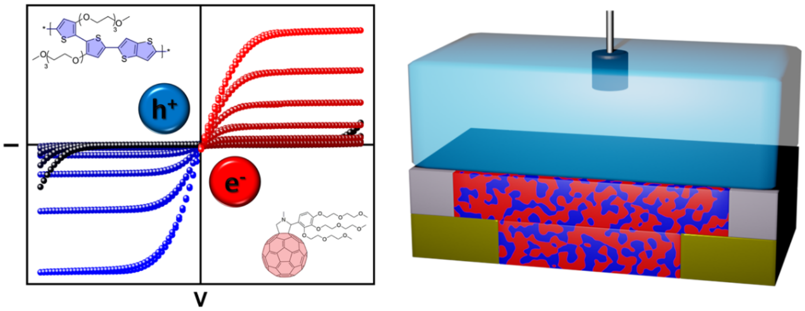
Biological signal detection and amplification has been a subject to intense research for the past few decades. However, coupling the ion-based biological signals to electron-based devices requires materials that support the transport of both ions and electrons, as well as circuit designs that are able to support on-site signal amplification. Organic mixed ionic-electronic conductors (OMIECs) are promising in this field because they can couple electronic and ionic currents, are easy to process into circuit architectures and offer mechanical compatibility with soft tissues. The most common and versatile device that utilizes OMIECs for the amplification of biological signals is the Organic electrochemical transistor (OECT) that relies on the injection/extraction of ions from an electrolyte into an OMIEC material to modulate its bulk conductivity [1].

Though most OMIECs are unipolar, namely p- or n-type, a rising group of ambipolar materials is a promising direction towards easy fabrication of complementary-like circuits as well as multi-ion detection and reduced footprint cofacial OECTs. To date, only a few ambipolar OMIECs have been demonstrated, most are homopolymers where the n- or p-type performance comes at the expense of the other. To overcome this limitation we suggested, for the first time, the use of blends to achieve ambipolarity in OMIECs [2].

In this work we demonstrate judicious selection of p- and n-type materials for ambipolar OMIECs as well as optimization of the blend ratio to achieve balanced performance. We studied a fullerene:polymer blend through a variety of characterization methods including optical and impedance spectroscopy, x-ray diffraction, OECTs, to gain insights on the structure-property relationships in the system. Our results show a significant effect of the blend ratio on device and spectral time constants, as well as preferential orientation of the molecular structure and gradual changes in the $\pi - \pi^*$ and lamellar stacking distances. All in all we show that the blend components act almost independently under the used methods and maintain with very good stability over 400 alternating sw … ay towards the design and fa … sors.



References
[1] Rashid, Reem B., Xudong Ji, and Jonathan Rivnay. "Organic electrochemical transistors in bioelectronic circuits." Biosensors and Bioelectronics 190 (2021): 113461.
[2] Stein, E., Nahor, O., Stolov, M. *et al.* Ambipolar blend-based organic electrochemical transistors and inverters. *Nat Commun* **13**, 5548 (2022).

O 2.5

Synthesis of (semi)conducting polymers in dispersed media

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Printed organic optoelectronic devices have recently gained importance and development due to their wide range of applications and techniques used. Printing techniques (*e.g.* inkjet, roll-to-roll, spray, screen printing, slot die, etc.) or coating techniques that use raw material in the form of inks are of major interest provided that the formulation steps of the compounds that constitute the different layers of the various devices are mastered and the rheology of the inks is adapted. In this field, the polymerizations in dispersed media (or heterogeneous polymerizations) can play a major role because they make it possible to obtain polymers and copolymers in a broad range of molar masses and sizes of particles in dispersing phases (going from the aqueous phase to more or less polar non-toxic solvents) compatible with the required technologies. Semiconducting polymer dispersions are already widely used in printed organic electronics and photovoltaics, namely poly(3,4-ethylene dioxythiophene) doped and stabilized with poly(styrene sulfonate), better known as PEDOT:PSS and used in aqueous dispersions. Not only have we revisited this ubiquitous system by replacing the polyanion and avoiding the use of additives to fine-tune the rheology of the inks to make them suitable for inkjet, screen printing, or slot die processes, but we have also applied miniemulsification or nanoprecipitation techniques to other classes of π-conjugated polymers. [1-6]

References

[1] A. I. Hofmann, W. T. T. Smaal, M. Mumtaz, D. Katsigiannopoulos, C. Brochon, F. Schütze, O. R. Hild, E. Cloutet, G. Hadziioannou, An alternative anionic polyelectrolyte for aqueous PEDOT dispersions: toward printable transparent electrodes, *Angew. Chem. Int. Ed.*, **54**, 8506-8510 (2015).
[2] A. I. Hofmann, D. Katsigiannopoulos, M. Mumtaz, I. Petsagkourakis, G. Pecastaings, G. Fleury, C. Schatz, E. Pavlopoulou, C. Brochon, G. Hadziioannou, E. Cloutet, How to Choose Polyelectrolytes for Aqueous Dispersions of Conducting PEDOT complexes, *Macromolecules,* **50**(5), 1959-1969 (2017).
[3] A. Glasser, E. Cloutet, G. Hadziioannou, H. Kellay, Tuning the Rheology of Conducting Polymer Inks for Various Deposition Processes, *Chem. Mater.* **31**(17), 6936-6944 (2019).
[4] L. Parrenin, C. Brochon, G. Hadziioannou, E. Cloutet, Low band gap semiconducting copolymer nanoparticles by Suzuki cross-coupling polymerization in alcoholic dispersed media, *Macromol. Rapid Commun.* **36**(20), 1816-1821 (2015).
[5] G. Prunet, L. Parrenin, E. Pavlopoulou, G. Pecastaings, C. Brochon, G. Hadziioannou, E. Cloutet, Aqueous PCDTBT:PC71BM photoactive inks made by nanoprecipitation, *Macromol. Rapid Commun.* **39**(2), 1700504 (2018).
[6] M. Geoghegan, M. M. Mróz, C. Botta, L. Parrenin, C. Brochon, E. Cloutet, E. Pavlopoulou, G. Hadziioannou, T. Virgili, Optical gain in semiconducting polymer nano and mesoparticles, *Molecules* **26**(4), pp. 1138 (2021).

O 2.6

Modeling cellular membrane potential using organic photovoltaic devices

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Traumatic Brain Injury (TBI) is a leading cause of disability and death, particularly among young adults. Encouraging outcomes observed in both preclinical and clinical investigations exploring neuromodulation techniques in the treatment of TBI lay a strong foundation for exploiting electrical stimulation as a means to restore function and alleviate trauma-induced disabilities [1], [2]. In the presented project we aim to develop the implementation of wireless photovoltaic devices for the treatment of TBI-induced disabilities. The recently developed organic electrolytic photocapacitors (OEPCs) consist of an ultrathin, transparent donor-acceptor bilayer of hydrogen-bonded pigments, phthalocyanine (H_2Pc, p-type), and N,N′-dimethylperylene-3,4:9,10-tetracarboxylic diimide (PTCDI, n-type), deposited on top of a back electrode [3]. The illumination unit consists of a high power LED with a peak wavelength of 660 nm and the appropriate illumination control circuit. We examined the potential of the OEPC devices to activate voltage-gated ion channels among different cell types, induce action potentials in cultured hippocampal neurons[4]. The effect of the OEPC devices was assessed using patch-clamp measurements, and comprehensive modeling and simulation methodologies. Following these promising results in the vitro studies, the first wireless electrodes were designed and implanted in an animal model.

Through elaborate in vitro testing and in silico simulations, we have attained promising evidence demonstrating the efficacy of our photovoltaic devices. Early experiments conducted in animal models have displayed encouraging outcomes. As we delve deeper into understanding the mechanisms behind this approach, our photovoltaic devices have the potential to improve TBI treatment. This could lead to better patient outcomes and a reduction in the overall impact of this condition.

Acknowledgment

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References

[1] S. Surendrakumar *et al.*, “Neuromodulation Therapies in Pre-Clinical Models of Traumatic Brain Injury: Systematic Review and Translational Applications.,” *J Neurotrauma*, vol. 40, no. 5–6, pp. 435–448, Mar. 2023, doi: 10.1089/neu.2022.0286.

[2] D. Ziesel *et al.*, “Electrical stimulation methods and protocols for the treatment of traumatic brain injury: a critical review of preclinical research,” *J NeuroEngineering Rehabil*, vol. 20, no. 1, p. 51, Apr. 2023, doi: 10.1186/s12984-023-01159-y.

[3] M. Silverå Ejneby *et al.*, “Extracellular Photovoltage Clamp Using Conducting Polymer- Modified Organic Photocapacitors,” *Adv. Mater. Technol.*, vol. 5, no. 3, p. 1900860, Mar. 2020, doi: 10.1002/admt.201900860.

O 2.7

Side chain engineering: the role of bulky substituents towards to original properties of organic optoelectronic materials

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Soluble organic optolectronic materials have a particular application potential for easily processed low-cost organic electronics devices. Solubility of organic π-conjugated small molecule derivatives, such as diketopyrrolopyrroles (DPPs), indigos, epindolidiones, squaraines and many others is usually attained by a side-chain alkyl substitution. Nowadays many organic semiconductors have been developed to improve the device performance, where most of the efforts focus on the design and synthesis of new π-conjugated backbones [1]. The alkyl side chain substitution of single molecules and polymer chains cause several important changes that are closely related to properties and directly to further use of π-conjugated systems. Adamantane and its derivatives are atypical fragments for side-chain alkyl substitution. However, adamantane is the simplest diamondoid, possesses exceptional physical characteristics and is the most stable saturated hydrocarbon isomer of such a small molecular weight. Above mentioned approach offers the synthesis of thermally stable and soluble high-performing materials for a wide range of organic electronics applications. The crucial component of the present approach is using adamantyl substitutions in solubilization side-groups. Ability of adamantane molecule to self-organize into crystals with unusually high melting point was used to reinforce packing of π-conjugated dyes in the solid state. Above mentioned side chain can improve solid-state fluorescence quantum yields of the materials [2, 3] and significantly increase the melting points. Considering electrical properties, as an example, a soluble DPP derivative with ethyl adamantyl side-groups showed abmipolar behavior with both hole and electron mobilities higher than the insoluble analogue [4]. Easily processable and convenient for upscaling and industrial processing, two novel thermodynamically stable regioregular poly-3- adamantylmethylthiophene and poly-3-adamantylethylthiophene polymers were investigated [5]. The prepared adamantane polythiophenes possess excellent thermal and chemical stability, which are important properties to produce stable and long-life devices.

References

[1] C. Wang, H. Dong, W. Hu, Y. Liu, D. Zhu, "Semiconducting π-Conjugated Systems in Field-Effect Transistors: A Material Odyssey of Organic Electronics", Chem. Rev., **112**, 4, 2208-2267 (2012).

[2] J. Krajcovic, A. Kovalenko, P. Heinrichova, M. Vala, M. Weiter, "Solid-state deep blue and UV fluorescent dyes based on para-bis(2-thienyl)phenylene", Journal of Luminiscence, **167**, 222-226 (2015).

[3] J. Krajcovic, A. Kovalenko, P. Heinrichova, M. Vala, M. Weiter, "Adamantyl side groups boosting the efficiency and thermal stability of organic solid-state fluorescent dyes", Journal of Luminiscence, **175**, 94-99 (2016)

[4] A. Kovalenko, C. Yumusak, P. Heinrichova, et al., "Adamantane substitutions: a path to high-performing, soluble, versatile and sustainable organic semiconducting materials", J.Mat.Chem. C, **5**, 4716-4723 (2017)

[5] J. Jancik, J. Pospisil, M. Kratochvil, J. Truksa, D. Altamura, C. Giannini, M. Weiter, D. Blasi, V. Lukes, E.D. Glowacki, J. Krajcovic, "Novel adamantane substituted polythiophenes as competitors to Poly (3-Hexylthiophene)", Polymer, **258**, 125274-125784 (2022)

O 2.8

Charge Transfer State Engineering for Tailor-Made Luminescent Organic Materials

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All-organic chromophores have found immense interest in current materials research. For the different purposes, color-specific, luminescent or non-luminescent, dissolved or aggregated chromophores are targeted. In order to achieve this, increasingly complex multi-channel photophysics are exploited, such as dual emission (DE), photoinduced electron transfer (PeT), RTP, TADF, TICT, or SLE/AIE in co-/crystals.[1] Charge transfer (CT) states play a central role in these processes. Tailor-made design of such compounds is thus of high technological demand; it requires, however, a detailed understanding to ultimately control the multiple deactivation processes, in particular the radiative and nonradiative decay channels, inter alia modulated by inter-chromophore interactions. The complexity of the underlying processes and their pivotal importance for materials' performance poses however grand challenges; in fact, misconceptions and false claims are frequently and increasingly found in this vivid area of research. A breakthrough in targeted design can be therefore only achieved in a holistic manner, combining advanced spectroscopic and computational methods in an intimate interdisciplinary 'dual expertise' scheme, in fact followed in our group.

The talk will give insight to our recent activities to decipher complex photophysics of organic materials involving CT states. This will include (i) exciplex-forming DE donor-acceptor triads for stimuli-responsive materials,[2] (ii) perylene-based deep-red solid state emitters through PeT regulation,[3] (iii) efficient TADF emitters for OLED vs. photocatalysis applications,[4] and (iv) solid state color regulation by intra- vs. intermolecular charge transfer (CT) states.[5] Following an overview on these processes, we will detail a selected example to illustrate the in-depth analysis procedure.

References

[1] For recent reviews, see (a) *Dual Emission: Classes, Mechanisms and Conditions*, S. K. Behera, S. Y. Park, J. Gierschner, Angew. Chem. Int. Ed. **2021**, 60, 22624; (b) *Luminescence in Crystalline Organic Materials: From Molecules to Molecular Solids*, J. Gierschner, J. Shi, D. Roca-Sanjuán, B. Milián-Medina, S. Varghese, S. Y. Park, Adv. Opt. Mater. **2021**, 9, 2002251.
[2] S. Feng, L. Wang, B. Milián-Medina, A. J. Meixner, M. Kwon, S. Y. Park, R. Wannemacher, J. Gierschner, *to be submitted*.
[3] N. Tang, J. Zhou, L. Wang, M. Stolte, G. Xie, X. Wen, L. Liu, F. Würthner, J. Gierschner, Z. Xie, Nature Commun. **2023**, 14, 1922.
[4] (a) Y. Kwon, J. Lee, Y. Noh, D. Kim, Y. Lee, C. Yu, J. C. Roldao, S. Feng, J. Gierschner, R. Wannemacher, M. S. Kwon, Nature Commun. **2023**, 14, 92; (b) S. Feng, J. C. Roldao, Y. Kwon, S. K. Behera, M. S. Kwon, B. Milián-Medina, R. Wannemacher, J. Gierschner, *to be submitted*.
[5] (a) S. Oh et al, J. Gierschner, S. Y. Park, J. Phys. Chem. C **2020**, 37, 20377; (b) I. Bhattacharjee, S. Kim, J. C. Roldao, S. Y. Park, B. Milián-Medina, R. Wannemacher, J. Gierschner, *to be submitted*.

O 2.9

Cellulose-Based Radiative Cooling and Solar Heating Powers Ionic Thermoelectrics

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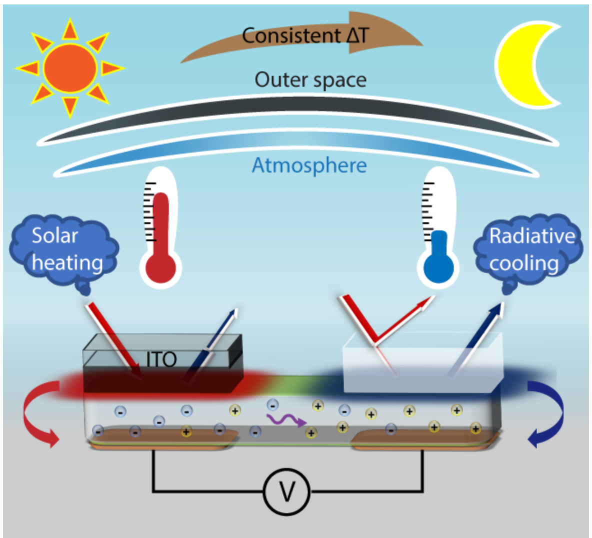
Cellulose opens for sustainable materials suitable for radiative cooling thanks to inherent high thermal emissivity combined with low solar absorptance. When desired, solar absorptance can be introduced by additives such as carbon black. However, such materials still show high thermal emissivity and therefore performs radiative cooling that counteracts the heating process if exposed to the sky. Here, this is addressed by a cellulose-carbon black composite with low mid-infrared (MIR) emissivity and corresponding suppressed radiative cooling thanks to a transparent IR-reflecting indium tin oxide coating. The resulting solar heater provides opposite optical properties in both the solar and thermal ranges compared to the cooler material in the form of solar-reflecting electrospun cellulose. Owing to these differences, exposing the two materials to the sky generated spontaneous temperature differences, as used to power an ionic thermoelectric device in both daytime and nighttime. The study characterizes these effects in detail using solar and sky simulators and through outdoor measurements. Using the concept to power ionic thermoelectric devices shows thermovoltages of >60 mV and 10 °C temperature differences already at moderate solar irradiance of ≈400 W m^{-2}.



Reference

[1] Liao, Mingna, et al. "Cellulose-Based Radiative Cooling and Solar Heating Powers Ionic Thermoelectrics." *Advanced Science* (2023): 2206510.

O 2.10

Charge-Transport Mechanisms in Desulfobubaceae Microbial Nanowires (Cable Bacteria)

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Charge transfer is fundamental to life, and organisms have developed various conductive structures to support vital processes. The distance of biological charge transport (CT) has long been thought to be limited to nm scale, yet recent studies suggest that electric currents can run along cm-long wires.[1-2] It is a fundamental challenge for scientists to understand the mechanisms of biological charge transfer in these extended structures, as biological materials are not usually associated with high conductivity. Furthermore, they could also bring potential future applications in microbial bio-electronics or even more in molecular electronics.[3] Several bacterial species have been found to produce conductive structures,[4] but the most studied are those of the *Shewanella* and *Geobacter* families, which produce external micron-sized nanowires and those of the *Desulfobubaceae* family which contain fibre-like structures within the cell membrane. Strings of these bacteria form cables and can transport charge over cm distances[5]; they are also referred to as cable bacteria. The wires under experimental research in this work are of the cable bacteria family. My theoretical study shed light on different CT mechanisms on cable bacteria and explain why these materials are so special as suggested by the experimental studies recently. Research by TU Delft professor Herre van der Zant' s research group has estimated high conductivity values for these bacteria which are the highest reported for any natural biological material (up to $79\ S\ cm^{-1}$).[5] They show that conduction through cable bacteria at high temperatures (100-300 K) follows an Arrhenius-type behavior with a low activation energy. As the temperature drops, the conductivity remains elevated and eventually stabilizes independent of temperature for moderate electric fields. The aim of this work is to shed light on the conductive mechanisms in these nanowires and to develop theoretical models that can describe conductance experiments in such microbial wires focusing on the bias-voltage, temperature and length dependence. Starting from our main motivation which is the experimental results of the TU Delft group,[5] through this work we create a theoretical framework consisting of different CT methods (based on incoherent classical and quantum hopping formalisms) that can describe such long-distance systems, explaining the transition through the different temperature regimes (classical and quantum). As far as we know, there is no comprehensive theoretical study of these experimental data. We derive parameters compatible with the experimental results while also providing a physical understanding of them. We also explain the role of the Ni-S group (part of the insulating protein layers of the cable bacteria) in the whole transport. Finally, we investigate the conditions that must be satisfied to reproduce such high conductivity values as in the experiments, and in a next step we propose ways to further enhance these value.

References

[1] G. Reguera, K. D. McCarthy, T. Mehta, J. S. Nicoll, M. T. Tuominen, D. R. Lovley, “Extracellular electron transfer via microbial nanowires,” Nature **435**, 1098-1101 (2005).
[2] Y. A. Gorby et al., “Electrically conductive bacterial nanowires produced by Shewanella oneidensis strain MR-1 and other microorganisms,” PNAS **106**, 11358-11363 (2006).
[3] N. S. Malvankar et al., “Tunable metallic-like conductivity in microbial nanowire networks,” Nature Nanotech **6**, 573–579 (2011).
[4] F. Wang et al., “Structure of Microbial Nanowires Reveals Stacked Hemes that Transport Electrons over Micrometers,” Cell **177**, 361-369 (2019).
[5] F. J. R. Meysman et al., “A highly conductive fibre network enables centimetre-scale electron transport in multicellular cable bacteria,” Nat Commun **10**, 4120 (2019).

O 2.11

Bio-inspired Approaches for Biotic/abiotic Interfaces in Intact Bacteria-based Biophotoelectrochemical Systems

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With the aim to convert solar energy into electrical energy, scientists and engineers have explored the possibility to couple abundant and sustainable photosynthetic biological catalysts with electrodes to mimic natural photosynthesis in a process that has been defined “semi-artificial photosynthesis”.[1] However, bacterial cells did not evolve to exchange electrons with an external electron acceptor/donor, making the transfer of photoinduced electron to (and from) an electrode the most critical challenge to be overcome.[2]

This talk will present the various bio-inspired approaches that we explored to tune the biotic/abiotic interface in intact bacteria-based biophotoelectrochemical systems. Specifically, the use of a polydopamine-purple bacteria-based redox-adhesive matrices enabling enhanced photocurrent production and bacterial cell attachment on electrodes will be discussed,[3] together with the possible use of bio-based electrode materials with polyhydroxybutyrate for improved bacteria-electrode interaction. Finally, the possible application of semi-artificial photosynthesis for the early monitoring of organic and inorganic pollutants will be presented.[4]

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References

[1] N. Kornienko, J.Z. Zhang, K.K. Sakimoto, P. Yang, E. Reisner, “Interfacing nature’s catalytic machinery with synthetic materials for semi-artificial photosynthesis”, Nat. Nanotechnology **13,** 890-899 (2018).
[2] L.D.M. Torquato and M. Grattieri, “Photobioelectrochemistry of intact photosynthetic bacteria: advances and future outlook”, Curr. Opin. Electrochem. **34**, 101018 (2022).
[3] G. Buscemi, D. Vona, P. Stufano, R. Labarile, P. Cosma, A. Agostiano, M. Trotta, G.M. Farinola, M. Grattieri, “Bio-Inspired Redox-Adhesive Polydopamine Matrix for Intact Bacteria Biohybrid Photoanodes”, ACS Appl. Mater. Interfaces **14**, 26631-26641 (2022).
[4] L.D.M. Torquato, R.M. Matteucci, P. Stufano, D. Vona, G.M. Farinola, M. Trotta, M.V. Boldrin Zanoni, M. Grattieri, “Photobioelectrocatalysis of Intact Photosynthetic Bacteria Exposed to Dinitrophenol”, ChemElectroChem **10**, e202300013 (2023).

O 2.12

Mixing and matching sustainable Melanin&Keratin from waste for green electronics

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In Italy the organic fraction is one of the most significant among municipal waste mainly processed for biogas production and incineration.[1] Other production activities such as the wool and poultry industries generate huge amounts of waste estimated as tons per year for wool and feathers.

Recently, the wet part of organic waste, the wool and feather waste have become an unexpected resource thanks to the sustainable extraction of biocompatible substances: the former with the reintegration of a natural melanin derived from the pupal exuviae of black soldier fly, the latter via keratin obtained from wool and feathers waste by sustainable processes. [2]–[4]

Natural melanins are ubiquitous pigments classified as: groups: eu/pheomelanine, neuromelanin, allomelanin, animal melanins.[5],[6] An intriguing class is the allomelanin (DHN) produced by fungi with radiotrophic properties capable of metabolizing γ radiation. [7] Melanin-based devices also show biodegradability with reduced phytotoxic effects, thus paving the way for green electronics. [8]

Keratin represents the most abundant structural protein in epithelial cells of animals. The extraction of keratin with different phases of purification appropriately modulated and depending on the origin (wool or feathers) leads to differentiation of their structure, allowing the production from membranes to gels making them interesting for microelectronics, in the medical field, and energy. [9], [10]

It is then realistic their reintegration into biosensors having specificity, sensitivity, and selectivity by taking advantage from melanin/keratin multifunctional properties. Here we show recent results on structural, chemical, and electrical characterizations of waste-derived keratin and melanin materials and their combination either in liquid phase or in device-like configuration as fundamental step to shed lights on all their possible functionalities for their exploitation in manufacturing, packaging, environmental technologies, medicine, and agriculture.

References

[1] ISPRA, *Rapporto Rifiuti Urbani*, vol. 53, no. 9. 2020.
[2] F. Salih, N. Memon, Z. Khatri, and S. Memon, *Environmental Technology & Innovation* 20, 2020, doi: 10.1016/j.eti.2020.101120.
[3] K. C. Surendra, et al., vol. 117, pp. 58–80, 2020, doi: 10.1016/j.wasman.2020.07.050.
[4] C. H. Kim *et al.*, *Processes*, vol. 9, no. 1, pp. 1–17, 2021, doi: 10.3390/pr9010161.
[5] M. D'Ischia *et al.*, *Pigment Cell Melanoma Res*, vol. 26, no. 5, pp. 616–633, 2013, doi: 10.1111/pcmr.12121.
[6] E. Di Mauro et al., " *MRS Commun*., vol. 7, no. 2, pp. 141–151, 2022, doi: 10.1557/mrc.2017.33.
[7] P. Manini *et al.*, *Chempluschem*, vol. 84, no. 9, pp. 1331–1337, 2019, doi: 10.1002/cplu.201900195.
[8] E. Di Mauro et al., *Nat Commun*, vol. 12, no. 1, pp. 1–10, 2021, doi: 10.1038/s41467-021-23227-4.
[9] A. B. Patil *et al.*, *Nanomicro Lett*, vol. 12, no. 1, 2020, doi: 10.1007/s40820-020-00459-5.
10] A. Shavandi, et al., *Biomater Sci*, vol. 5, no. 9, pp. 1699–1735, 2017, doi: 10.1039/c7bm00411g.

O 2.13

The Photophysics of Cell Membrane-Targeting Phototransducers

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In the last years, the use of light as a tool for modulating membrane potential and bioelectricity has emerged as a fascinating opportunity, with the broad aim of establishing life-machine symbiosis that can help in healing disorders and restoring biological functions. An approach to induce light sensitivity in animal cells, which are usually transparent to visible light, is the use of photoactuators. These are photoactive materials that can decorate or localize into the cell membrane and are able to transduce light into a signal that can be processed by the cells. A variety of materials are suitable for the non-genetic optostimulation of cells, ranging from inorganic nanoparticles to organic polymer films and nanostructures.

In this work, I make use of different small membrane-targeting molecules. The cell membrane and its electrical potential represent the core of bioelectricity, hence constituting an ideal target for exogenous modulation of signalling. The study unveils the photostimulation mechanism, intending to link the photophysical changes occurring in the molecular photoactuator after light absorption, to the different biological effects on *in vitro* cell models.

Evaluating the photoinduced effects of the photoactuators on different cell models, including HEK-293 cells, primary neurons and bacteria strains, and correlating them with the photophysical characterization of the aforementioned molecules, lead us to identify different light-driven mechanisms that allow us to control and manipulate the cell activity.

The photoinduced effects observed on cells are found to be related, for instance, (*i*) the thinning or thickening of the membrane due to conformational changes in the molecules, (*ii*) the increase of the membrane permeabilization, and the formation of pore-like structures likely due to the lipid peroxidation following the photosensitization of singlet oxygen within the cell membrane, (*iii*) the rearrangement of the charges adsorbed to the membrane due to variations in the molecular dipole moment.

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On the Coupling Mechanism Occurring at the Neuron-Nanoparticle Interface

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The injection of organic photo-responsive nanoparticles (NPs) of poly(3-hexyltiophene) (P3HT) into rat models of retinitis pigmentosa was proposed as a "*liquid retina device*" to treat degenerative blindness, inducing a light evoked retinal neuron response[1,2]. Although the efficiency of organic polymer-based retinal devices in vivo has been proven, the interpretation of the working mechanisms that grant photostimulation at the polymer/neuron interface is still a matter of debate. In the present work, we focus on understanding the mechanisms which may play a role at the bio-hybrid interface, decoupling them into: (i) a faradaic effect, which in our case consists in the photocathodic behavior of P3HT in watery oxygenated environment; (ii) a capacitive effect, due to light induced capacitive charging of the NP. With mathematical modeling and electrochemical studies, we are able to identify the relative importance of each mechanism as a function of light intensity impinging onto the substrate, cleft size and cleft resistive properties.

The faradaic mechanism, connected to the production of O_2^- in the cleft, appears to be relevant solely when light intensity increases above the physiological ranges. The capacitive effect induced by the electrostatic charging of the NP is instead appreciable only in the presence of a highly resistive medium, where ionic screening can be assumed as negligible (Debye Length>>cleft thickness): if this condition is verified by the system, even physiological light intensities (0.2 W/m^2) are able to induce appreciable depolarization of the neurons. The highly resistive medium in the model is accounted for by the presence of adhesion proteins in the cleft. Therefore, the formation of *"proteic islands"* is suggested by the model as a fundamental ingredient to ensure the coupling among neuron and nanoparticle at reduced light intensity. Preliminary confirmations to the model come from ex vivo experiments on retinal explants that received P3HT-NPs in the subretinal space either acutely after the explantation or that were taken from rats which had been subretinally injected in vivo with P3HT-NPs one month before. The recordings of retinal ganglion cell firing on acutely injected explants displayed a significantly reduced response with respect to the retinas which experiences a prolonged in vivo contact with the NPs before explantation. The combined use of modeling and physiological experiments suggests that, in vivo, NPs are engulfed by the neuronal membrane with a highly resistive medium which ensures an efficient capacitive coupling. While at the high light intensities used in in vitro experiments both phenomena may take place, at the lower light intensities used in vivo the sole capacitive effect is responsible for the photostimulation.

References

[1] Maya-Vetencourt, J.F., Manfredi, G., Mete, M. et al. Subretinally injected semiconducting polymer nanoparticles rescue vision in a rat model of retinal dystrophy. Nat. Nanotechnol.15, 698–708 (2020). https://doi.org/10.1038/s41565-020-0696-3

[2] Francia, S., Shmal, D., Di Marco, S. et al. Light-induced charge generation in polymeric nanoparticles restores vision in advanced-stage retinitis pigmentosa rats. Nat Commun13, 3677 (2022). https://doi.org/10.1038/s41467-022-31368-3

O 2.15

The Effects of Strain on the Electronic Properties of Rubrene Single Crystals

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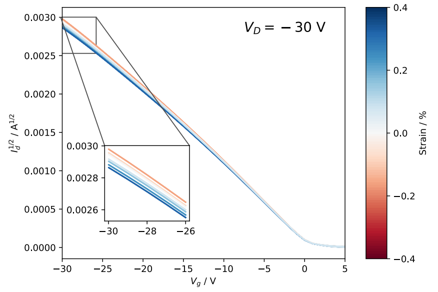
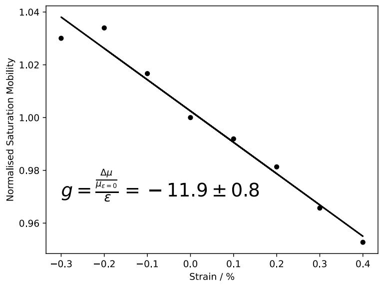
Small molecule organic semiconductors have the potential to create the next generation of flexible electronics - key for industries such as biomedical sensing and wearables - due to their inherently soft mechanical properties and compatibility with flexible substrates. However, for these devices to be used in practical applications it must be understood how the bending process affects the electronic properties: on one hand, devices must be tolerant to strain in order to keep functioning during flexure, but it is also desirable to have semiconductors that have variable conductivity to act as strain sensors.

More fundamentally, strain dependent measurements can give an indication of how charge transport works in organic semiconductors, where there is a complex interplay between the band-like transport and the thermal vibrations which have the potential to disrupt or enhance carrier motion, due to being on a similar energy scale. Applying strain allows one to alter the band structure (through changing intermolecular distances) as well as changing the amplitude of vibrational modes, without changing the molecule or crystal structure itself, which can act as a confounding variable. Single crystals act as a model system to investigate these changes due to the relatively high order and lack of defects such as grain boundaries. Rubrene single crystals have been shown to have record high mobility (up to 20 cm^2/Vs)[2] and have shown to have a large variation of mobility with strain (up to 100 % per % strain applied) so are the semiconductor of choice to observe any changes in the various properties studied [3].

In this work we have developed a novel method for applying a consistent strain with micrometre precision to rubrene single crystals whilst measuring them in an FET geometry. In addition, we have the capability to insert the system into a cryostat to investigate the temperature dependence of any effects. With this method we are able to measure the strain dependence of important electronic properties such as the mobility and the Seebeck coefficient (which has never previously been reported), giving key insight into the charge transport mechanism in these materials. Preliminary results from these experiments have shown repeatable and reversible variation over 10 % in mobility – see figures below.





It is hoped that the results of these studies will provide further insight into how charge transport in rubrene is modulated by the interplay between the static energetic landscape provided by the transfer integrals between adjacent molecules and the off-diagonal energetic disorder provided by the vibrations throughout the crystal. There are also important questions to be answered about the wide variation in the magnitude of any effects seen, with this study adding more vital data to a growing understanding of this important property.

References

[1] S. Fratini, M. Nikolka, A. Salleo, G. Schweicher and H. Sirringhaus, *Nature Materials*, 2020, **19**, 491–502.
[2] J. Takeya *et. al.*, *Appl. Phys. Lett.*, 2007, **90**, 102120.
[3] H. H. Choi *et. al.*, *Advanced Science*, 2020, **7**, 1901824.

O 2.16

2D-Materials and Hydrogels based Triboelectric Nanogenerators (TENGs) for Energy Harvesting and Self-Powered Tactile Sensors

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The increasing demand for novel wearable, flexible, conformable devices and sensors has boosted the search for alternative sustainable energy sources. Such largely distributed and off-grid devices and sensors, are often powered by batteries that are mostly produced from toxic and hazardous materials. However, advances in new low power technologies, as the one largely developed for the internet of Things (IoT), wearable and portable electronics, require only few tens of μW up to few mW of power supply to operate. Such low power allows for their sustainable integration with energy harvesters that can scavenge the wasted environmental energy. Between mechanical energy harvesters, triboelectric nanogenerator (TENG) have gained increasing attention as novel low-cost and green energy solution. They can efficiently convert the widely distributed and dispersed mechanical energy into a sustainable electrical power source. Unlike other mechanical energy harvesters, as piezoelectric and electromagnetic generators, TENGs are typically fabricated from non-toxic, biodegradable, recyclable materials using scalable fabrication processing. [1, 2] In addition, TENGs can efficiently operate also in the low frequency range and can be designed to operate as self-powered motion and pressure sensors. This aspect hugely widens their potential impact in a variety of application fields spanning from wind and sea wave energy harvesting (blue energy) to wearables, soft-robotics and artificial skin.[3]

TENGs energy conversion mechanism relies on the charge transfer which occurs between two materials placed under friction forces and that own different electron affinities. Different strategies to increase the surface triboelectrification through chemical modification or surface patterning have been proposed. Here, we will show how the electrode work function and capacitance are relevant factors to be considered for improving TENGs power output, a main aspect which has often been disregarded in previous work. [4,5]

We will also highlight the fundamental role played by the optimal engineering of the interface between the triboelectric material and the electrode by the introduction of 2D-materials and 2D-transistion metal dichalcogenides.[6] Additionally we will provide novel insights on the material composition-function-structure relationship, necessary for the design of novel hydrogels to be integrated into TENGs based tactile sensors. The specific role of composition, structure and electrolytic capacitance of hydrogel based on polyvinyl alchool derivatives will be highlighted, and clarified. Overall, work intends to provide useful guidelines for the future design of new materials and device architecture that can lead to improved TENGs performances, fostering their sooner integration into novel low power and sustainable technologies.

References:

[1] Y. Zi, H. Guo, Z. Wen, M. H. Yeh, C. Hu and Z. L. Wang, ACS Nano **10**, 4797–4805 (2016).
[2] G. *Pace, M. Caironi, Nano Energy 108, 108168 (2023)
[3] C. Wu, A. C. Wang, W. Ding, H. Guo and Z. L. Wang, Adv. Energy Mater. **9**, 1–25 (2019).
[4] G. *Pace, F. Bonaccorso, Nano Energy **76**, 104989 (2020).
[5] G. *Pace, F. Bonaccorso, Nano Energy **87**, 106173 (2021).
[6] G. *Pace, F. Bonaccorso, Advanced Materials **2211037** (2023).
[7] G. *Pace, M.Lavorgna, P. Basset, submitted Nano Energy (2023)

O 2.17

Ellipsometric measurements in organic semiconducting materials for photovoltaics

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Organic semiconducting materials are attracting considerable attention due to their mechanical flexibility, easy processing, potentially low cost, recyclability and easy tuning of their optoelectronic properties, making them interesting for applications in scalable electronics e.g. solar cells, light emitting diodes, and photodetectors [1]. The understanding of the correlation between the material structure and its optical and electrical properties, is a vital requirement for performance modeling as well as for design optimization of optoelectronic devices. The most important optical parameter that governs the behaviour of optoelectronic devices is the refractive index of the materials involved and thus an accurate determination of this parameter is crucial for the development of technology. Precisely, spectroscopic ellipsometry (SE) is a non-invasive and highly sensitive technique for the determination of optical constants and thicknesses of thin films [2].

In this study, we implemented variable-angle spectroscopic (1.2 – 5.4 eV) ellipsometry (VASE) to determine the refractive index (n), extinction coefficient (k), and thickness of different thin films of organic materials deposited by blade coating onto glass substrates. We selected 5 wide bandgap materials, interesting for indoor photovoltaics and for tandem solar cells. The ellipsometric data was analyzed using an electronic model based on the Tauc-Lorentz (TL) oscillator, as it leads to accurate fits of the optical functions of our materials. The thicknesses deduced by these fits are in the range of ca. 16 to 146 nm, which is in good agreement with those obtained using surface profilometry, and the calculated absorption spectra using the optical constants match those measured by spectrophotometry. The aim of this study is to demonstrate the potential of ellipsometry towards the determination of the optical properties of organic semiconductors, that will be followed by numerical simulations in the future, allowing us to model appropriately the performance of optoelectronic devices based on these materials.

References

[1] Y. Zhou and C. Wang, “Organic optoelectronics creating new opportunities for science and applications”, Frontiers of Optoelectronics 15, 51 (2022).

[2] M.I. Alonso and M. Campoy-Quiles, “Conjugated Polymers: Relationship Between Morphology and Optical Properties” in *Ellipsometry of Functional Organic Surfaces and Films*. K. Hinrichs, KJ Eichhorn, eds. (Springer Series in Surface Sciences, vol 52., Springer, Cham., 2018).

O 2.18

Towards a Deeper Understanding of the Ionic Charging in Naphthalenediimide-Based N-Type Conjugated Polymer Electrodes

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Conjugated polymers with hydrophilic side chains are a type of organic mixed ionic/electronic conductors (OMIECs) that is attracting interest for applications in organic electrochemical transistors, electrochromic devices and energy storage devices. Compared with numerous stable and high-performance p-type mixed-conducting polymers, n-type mixed-conducting polymers usually suffer from poor stability in water and air. To date, most reported solution processable n-type mixed conducting polymers that show good stability, high electron mobility and high specific capacity, involve the naphthalenediimide (NDI) unit. [1-3] However, NDI-based mixed-conducting polymers vary in their performance and their mechanical and electrochemical stability with varying molecular designs and electrolyte choice. The underlying mechanisms by which polymer side chains and backbones facilitate ion/electron transport and storage, and by which ionic charging/discharging deteriorates the stability are not fully understood. Thus, to identify the microscopic interactions controlling the overall performance and extract design rules for further material and device optimisation, *operando* characterisation methods and multiscale models are required. In this work, we study several NDI-based n-type mixed conducting polymers with different side chain and backbone structures operating in aqueous electrolytes of systematically varying concentrations to control both the mechanical and electrochemical stabilities. We observe that increasing electrolyte concentration and replacing a small fraction of hydrophilic side chains with hydrophobic ones largely improve the performance and stability of the NDI-based n-type mixed conducting polymers. This improvement can be tentatively attributed to a reduction in swelling, which avoids excessive electrolyte uptake, thereby improving the environment for ion transport and maintaining the intermolecular connections. We propose design rules for both material and electrolyte to maximise reversible multi-electron charging of n-type mixed conducting polymers.

References

[1] D. Moia, "Design and evaluation of conjugated polymers with polar side chains as electrode materials for electrochemical energy storage in aqueous electrolytes", *Energy Environ. Sci.* **12**, 1349-1357 (2019).

[2] I. P. Maria, "The Effect of Alkyl Spacers on the Mixed Ionic-Electronic Conduction Properties of N-Type Polymers", *Adv. Funct. Mater.* **31**, 2008718 (2021).

[3] A. A. Szumska, "Reversible Electrochemical Charging of n-Type Conjugated Polymer Electrodes in Aqueous Electrolytes", J. Am. Chem. Soc. **143**, 14795-14805 (2021).

O 3.1

Resonant Tender X-ray Scattering of Conjugated Polymers

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In this presentation I will discuss the development and application of resonant tender X-ray scattering to study the microstructure of conjugated polymers,[1] see Fig. 1. Most conjugated polymers are semicrystalline, with the way in which polymer chains pack strongly affecting their optoelectronic performance. Unlike small molecule crystals whose structure can be directly solved using crystallographic methods, conjugated polymers are more disordered meaning that there are not enough diffraction peaks available. To squeeze more information from the diffraction peaks that are present, we have turned to resonant diffraction: By varying the X-ray energy across an elemental absorption edge, the variations in diffraction intensity that are observed can provide additional information. Also known as anomalous diffraction, this technique has been applied in other fields including protein crystallography. As many conjugated polymers utilise sulfur as heteroatoms, we have studied resonant diffraction effects at the sulfur K-edge in the tender X-ray regime.[2-4] Such measurements enable different crystalline polymorphs to be distinguished,[2] and provide unambiguous determination of the titling of the conjugated backbone within the unit cell.[3, 4] Performing X-ray scattering at tender X-ray energies is also shown to be able to provide enhanced contrast for small angle X-ray scattering measurements,[5] with strong potential for further applications such as determining the location of counterions in doped conjugated polymers.[6]

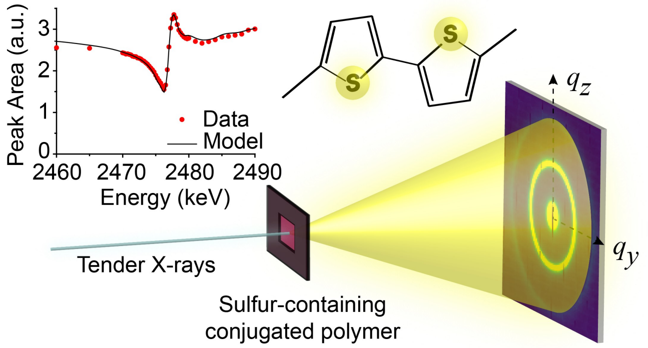

Fig.1. Schematic of a resonant tender X-ray scattering experiment.

References

[1] C. R. McNeill, Acc. Mater. Res. **16**, 4, 16-26 (2023).

[2] G. Freychet, E. Gann, L. Thomsen, X. Jiao, C. R. McNeill, “Resonant Tender X-ray Diffraction for Disclosing the Molecular Packing of Paracrystalline Conjugated Polymer Films,” J. Am. Chem. Soc. **143**, 1409-1415 (2021).

[3] G. Freychet, E. M. Zhernenkov, C. R. McNeill, “Anisotropic Resonant X-ray Diffraction of a Conjugated Polymer at the Sulfur K-edge” J. Chem. Phys. Lett. **12**, 3762-3766 (2021).

[4] G. Freychet et al., “Resolving the backbone tilt of crystalline poly (3-hexylthiophene) with resonant tender X-ray diffraction” Mater. Horiz. **9**, 1649-1657 (2022).

[5] G. Freychet et al., “Drastic Enhancement of X-ray Scattering Contrast between Amorphous and Crystalline Phases of Poly (3-hexylthiophene) at the Sulfur K-Edge,” ACS Materials Lett. **4**, 764-769 (2022).

[6] L. Q. Flagg et al., “Resonant X-ray Diffraction Reveals the Location of Counterions in Doped Organic Mixed Ionic Conductors,” Chem. Mater. https://doi.org/10.1021/acs.chemmater.3c00180 (2023).

O 3.2

Electrically and mechanically decoupled single chromophores by tripodal scaffolds on gold: Towards Organic Optoelectronic Devices

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Control of the molecular arrangement and spatial orientation of light-emitting molecules on metallic surfaces is of crucial importance for the construction of artificial photonic devices such as organic light-emitting diodes or single photon sources for quantum optical technologies. Our approach to achieve both an efficient decoupling of molecular chromophore and the spatial arrangement of functional molecules on gold surfaces is based on rigid multipodal scaffolds [1]. Series of functional molecular tripods based on tetraphenylmethane foot-structures have been prepared in order to analyze their arrangement and to investigate the mechanical and/or chemical manipulation of the protruding chromophore. Our particular focus is set on tripodal naphthalene diimide (NDI) chromophores with the intention to tune their optical properties by NDI-core substitution at the positions 2,6 and maintain their electronic decoupling [2]. In total, three types of NDI-chromophores were prepared and studied on two different molecular platforms. The orientation of molecules on gold has been studied after spray deposition by means of a low temperature UHV-STM technique with electroluminescence setup. Extensive low temperature STML studies of NDI molecules on the small tripodal platform deposited on Au(111) revealed that at most a minority of the tripodal chromophores are standing upright and show electroluminescence, while the majority are lying flat on the gold substrate [2]. Moreover, we show that fully quenched NDI molecules on a Au(111) surface can be manipulated with the STM tip to decouple the relevant frontier orbitals from the metallic substrate and thus switch a single molecule to a light emitting state [3]. While NDI-chromophores on extended tripodal scaffolds are standing exclusively upright on Au(111) and thus enables both, efficient electrical and mechanical decoupling of individual chromophores from metallic leads [4]. The single molecule junction has an impressive efficiency of 10^{-3} photons per electron and is robust enough to allow for detailed STML experiments, including photon maps of an individual molecule. Furthermore, the chromophore mounted on the extended tripodal scaffold is also mechanically decoupled, increasing the lifetime of vibrational excited states indicated by hot luminescence bands for the first time. Our work thus opens up avenues for further applications of surface mounted molecular devices and benefits from the possibility to functionalize such modular extended tripodal scaffold with functional subunits to form mechanically stable contact and control the spatial arrangement of the protruding functionality on metallic substrates in order to exploit their optical, magnetic and mechanical features.

References

[1] Valášek M.; Mayor M. Chem. Eur. J. **23**, 13538–13548 (2017).
[2] Balzer N.; Lukášek J.; Valášek M.; Rai V.; Sun Q.; Gerhard L.; Wulfhekel W.; Mayor M. Chem. Eur. J. **27**, 12144–12155 (2021).
[3] Rai V.; Gerhard L.; Balzer N.; Valášek M.; Holzer C.; Yang L.; Wegener M.; Rockstuhl C.; Mayor M.; Wulfhekel W. Phys. Rev. Lett. **130**, 036201 (2023).
[4] Rai V.; Balzer N.; Derenbach, G.; Holzer C.; Mayor M.; Wulfhekel W.; Gerhard L.; Valášek M. *under review*.

O 3.3

Quantitative characterisation of conjugated polymers: mass distribution and polymerisation defects determined by molecular scale imaging

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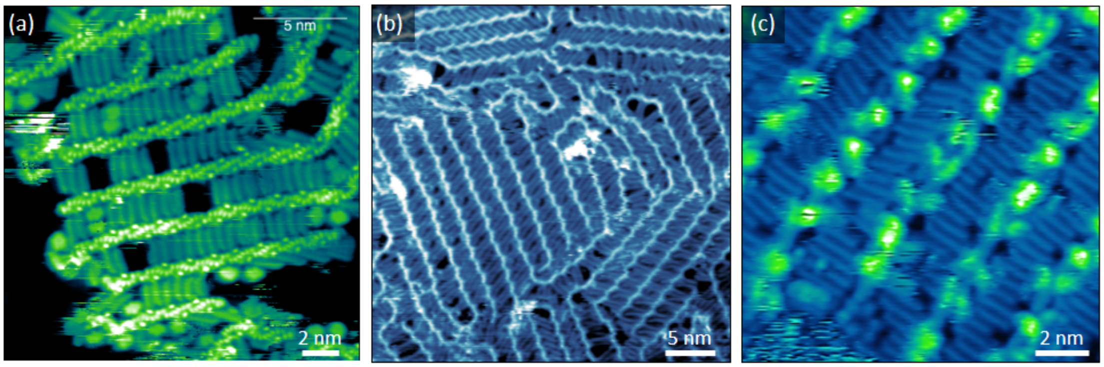
In this talk I will demonstrate that high resolution scanning tunnelling microscopy (STM) is capable of delivering crucial information — that cannot be achieved by other current analytical method — about “real world” electronic and energy materials. In particular, I will show that by combining vacuum electrospray deposition (ESD) and high-resolution STM, it is possible to image conjugated polymers used in organic (bio)electronics and photovoltaic devices with unprecedented details.

Based on this, it becomes possible to sequence the polymers by visual inspection and to determine their molecular mass distribution by simply counting the repeat units. I will further show that we can precisely establish the nature and frequency of synthetic defects in the polymer backbone and determine the polymer assembly motifs with sub-molecular spatial resolution.[1-5] By benchmarking the results of ESD-STM against NMR, SEC, XRD and mass spectrometry, I will demonstrate that our new technique successfully reproduces and extends the analytical power of tradition characterisation methods.



High-resolution STM image of (a) poly(C_{14}DPPF-F), (b) pBTTT, and (c) IDT-BT on Au(111)

References

[1] D.A. Warr, *et al.,* “Sequencing conjugated polymers by eye” *Sci. Adv.* **4**, eaas9543 (2018).

[2] H. Chen, *et al.,* “The Effect of Ring Expansion in Thienobenzo[b]indacenodithiophene Polymers for Organic Field-Effect Transistors” *J. Am. Chem. Soc.* **141**, 18806 (2019).

[3] M. Xiao, *et al.,* ”Anisotropy of charge transport in a uniaxially aligned fused electron deficient polymer” *Adv. Mater.* **32**, 2000063 (2020).

[4] R.K. Hallani, *et al.,* ”Regiochemistry-driven Organic Electrochemical Transistor Performance Enhancement in Ethylene Glycol Functionalized Polythiophenes” *J. Am. Chem. Soc.* **143**, 11007 (2021).

[5] S. Moro, *et al.,* ”The Effect of Glycol Side Chains on the Assembly and Microstructure of Conjugated Polymers” *ACS Nano* **16**, 21303 (2022).

O 3.4

How Does Antiaromaticity Affect Single Molecule Conductance?

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The question of how aromaticity and antiaromaticity influence molecular conductance is not straight forward to answer. To compare compounds with varying degrees of aromaticity/antiaromaticity, the structures should be similar enough that other effects, such as size differences, substituent effects or changes in the molecule's charge can be ignored. In order to mitigate this as much as possible, we have designed and measured several compounds containing an aromatic anthracene unit and compared them with analogous antiaromatic, non-alternant, dibenzopentalene compounds. Both compounds have similar sized π-systems with the same number of π-bonds between the anchoring groups, making it as fair a comparison as possible. For the SMe-anchored compounds, there is almost no difference in conductance between anthracene and dibenzopentalene,[1] despite the prediction that aromaticity should hinder conductance versus antiaromaticity.[2] Conversely, for the pyridyl-anchored compounds, there is a noticeable conductance enhancement for the dibenzopentalene over the anthracene. We explain this behavior in terms of the level alignment of each molecule with respect to the Fermi level. Antiaromaticity tends to promote a lower-lying LUMO level, which assists the conductance of the pyridyl-anchored molecules.

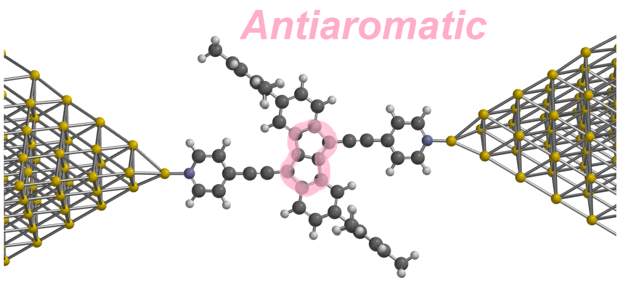

Figure. Single molecule junction containing an antiaromatic dibenzopentalene.

References

[1] Schmidt, M.; Wassy, D.; Hermann, M.; González, M. T.; Agrãit, N.; Zotti, L. A.; Esser, B.; Leary, E. Single-Molecule Conductance of Dibenzopentalenes: Antiaromaticity and Quantum Interference. Chem. Commun. 2021, 57 (6), 745–748.
[2] Breslow, R.; Foss, F. W. Charge Transport in Nanoscale Aromatic and Antiaromatic Systems. J. Phys. Condens. Matter 2008, 20 (37), 374104.

O 3.5

Non-Conjugated Polymeric and Dimeric Acceptors for Efficient Polymer Solar Cells

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High efficiency and mechanical robustness are both crucial for the practical applications of all-polymer solar cells (all-PSCs) in stretchable and wearable electronics.[1] In this regard, a series of new polymer acceptors (P_As) is reported by incorporating a flexible conjugation-break spacer (FCBS) to achieve highly efficient and mechanically robust all-PSCs. Incorporation of FCBS affords the effective modulation of the crystallinity and pre-aggregation of the P_As, and achieves the optimal blend morphology with polymer donor (P_D), increasing both the photovoltaic and mechanical properties of all-PSCs.[2] In particular, an all-PSC based on PYTS-0.3 P_A incorporated with 30% FCBS and PBDB-T P_D demonstrates a high power conversion efficiency (PCE) of 14.68% and excellent mechanical stretchability with a crack onset strain (COS) of 21.64% and toughness of 3.86 MJ m^{-3}, which is significantly superior to those of devices with the P_A without the FCBS (PYTS-0.0, PCE = 13.01%, and toughness = 2.70 MJ m^{-3}). In a follow up work, we have investigated the influence of the length of flexible spacer. It was found that the polymer acceptor with shorter spacer achieved the highest performance.[3] These results reveal that the introduction of FCBS into the conjugated backbone is a highly feasible strategy to simultaneously improve the PCE and stretchability of PSCs. Dimeric acceptors may carry the advantages of both small molecular and polymeric acceptors, but circumventing their disadvantages. The synthesized dimers in this work exhibit different conformations (O- and U-shape), enabling control over the molecular packing, layer morphology and, ultimately, the solar cell performance. The O-shaped dimer exhibits a more coplanar conformation with an upshifted lowest unoccupied molecular orbital energy level, enhanced light absorption, tighter π-π stacking and a more ordered molecular packing motif, and better miscibility with the donor polymer PM6 compared with its U-shaped analogue. Optimized PSCs based on PM6 and this dimer deliver a maximum power conversion efficiency (PCE) of 18.09%. We demonstrate the important role of molecular conformation of the acceptor components and highlight the potential of dimeric acceptors to improve the performance of PSCs

References

[1] Q. Fan, W. Su, S. Chen, T. Liu, W. Zhuang, R. Ma, X. Wen, Z. Yin, Z. Luo, X. Guo, L. Hou, K. Moth-Poulsen, Y. Li, Z. Zhang, C. Yang, D. Yu, H. Yan, M. Zhang, E. Wang, *Angew Chem Int Ed Engl* **2020**, *59*, 19835-19840.
[2] Z. Genene, J.-W. Lee, S.-W. Lee, Q. Chen, Z. Tan, B. A. Abdulahi, D. Yu, T.-S. Kim, B. J. Kim, E. Wang, *Adv. Mater.*, **2022**, *34*, 2107361
[3] Q. Chen, Y. H. Han, L. R. Franco, C. F. N. Marchiori, Z. Genene, C. M. Araujo, J.-W. Lee, T. N.-L. Phan, J. Wu, D. Yu, D. J. Kim, T.-S. Kim, L. Hou, B. J. Kim, E. Wang, *Nano-Micro Letters* **2022**, *14*, 164.

O 3.6

Controlled Doping of the Active Layer as a possible Performance Enhancer in Organic Solar Cells

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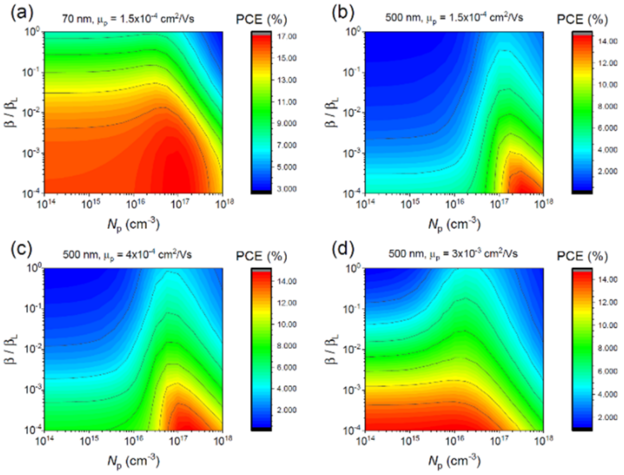
Intentionally doped organic semiconductors are frequently used in both organic and Perovskite solar cells as interlayers between the contacts and the active (light absorbing) layer; so-called charge transport layers. By introducing molecular dopants to the charge transport layer, one can control the Fermi level and thus achieve Ohmic injection and barrier free extraction of charges, provided that the doping concentration is high enough. However, common knowledge in the field suggests that doping of the active layer is detrimental for device performance and as such undesirable. When the doping concentration is high enough, the potential drop in the device will occur over the depletion region leaving the rest of the device mostly charge-neutral and field-free. In this case, charges generated in the depletion region will be efficiently extracted whereas those generated in the neutral region will predominantly recombine, which will lead to a voltage dependent photocurrent and a concomitant negative effect on the FF [1].

In a recent publication, we have shown that contrary to earlier results, doping of the active layer is not always bad for performance. We use electro-optical simulations based on a drift-diffusion approach combined with experimental characterization of a strongly absorbing organic solar cell blend to demonstrate that doping can in fact have a positive effect on device performance [2]. The increased efficiency is achieved by:
i) optimizing the induced depletion width to the charge generation region for efficient charge generation, and
ii) increasing the charge collection by increasing the conductivity of the charge carrier that needs to transport to the non-transparent electrode.



References

[1] O. J. Sandberg, S. Dahlström, M. Nyman, S. Wilken, D. Scheunemann, R. Österbacka, *Phys. Rev. Applied* **12**, 034008 (2019)

[2] M. Nyman, O. J. Sandberg, W. Li, S. Zeiske, R. Kerremans, P. Meredith, and A. Armin, *Solar RRL* **5 (5)**, 2100018 (2021)

O 3.7

Degradation Mechanism and Stability Improvement of Organic Solar Cells

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Power conversion efficiency of organic solar cells (OSCs) has reached over 19% for single junction cells. Stability is therefore become the next most important issue before the commercialization of OSCs. Various degradation pathways, including materials decomposition of materials by O_2/H_2O, morphology changes of the photoactive layers during operation have been clarified. By comparing the influence of ZnO on the stability of the polymer:non-fullerene acceptor (NFA) solar cells, we confirmed that photon-induced decomposition of NFA at the ZnO interface caused the fast performance decay of the high-performance polymer:NFA solar cells, where photon oxidation of the dangling hydroxy anions on ZnO surface to the reactive hydroxy radicals is the basic chemical reasons (Figure 1a).[1] Surface passivation of ZnO with Lewis acids significantly improved device stability.[2] In addition, formation of an atom cage between the β-alkyl side chain and the C=C bond prevents the attack hydroxyl radicals and consequently improves the photo stability of the cells (Figure 1b).[3] With these, high-performance (with PCE over 17%) and stable (with T_{80} > 6000 hours) cells were prepared. We will also report our efforts in developing solution-processed thin film encapsulation results.

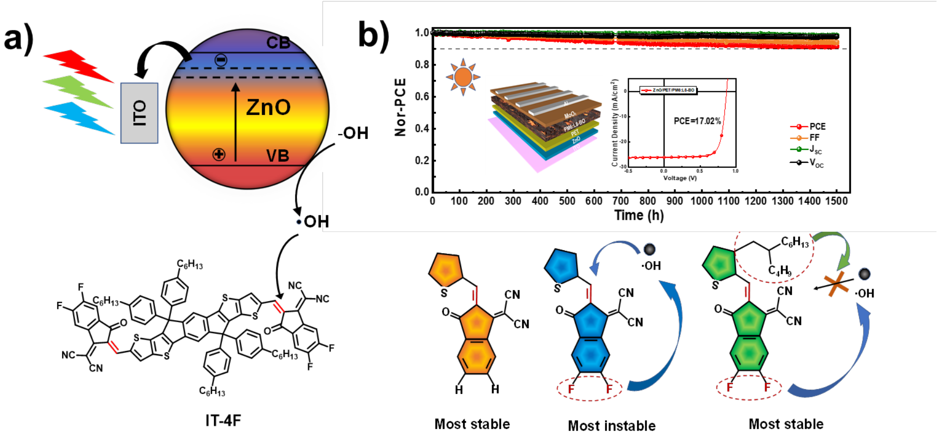

Figure 1. a) Photon decomposition of NFA at the ZnO interface; b) protecting the C=C from the attack of the reactive hydroxyl radicals to improve device stability.

References

[1]. Bowen Liu, Yunfei Han, Zerui Li, Huimin Gu, Lingpeng Yan, Yi Lin, Qun Luo, Shangfeng Yang, and Chang-Qi Ma, "*Visible Light-Induced Degradation of Inverted Polymer:Non-Fullerene Acceptor Solar Cells: Initiated by the Light Absorption of ZnO Layer*" Solar RRL **5** (1), 2000638 (2021).

[2]. Yunfei Han, Huilong Dong, Wei Pan, Bowen Liu, Xingze Chen, Rong Huang, Zhiyun Li, Fangsen Li, Qun Luo, Jianqi Zhang, Zhixiang Wei, and Chang-Qi Ma, "*An Efficiency of 16.46% and a T80 Lifetime of Over 4000 h for the PM6:Y6 Inverted Organic Solar Cells Enabled by Surface Acid Treatment of the Zinc Oxide Electron Transporting Layer*," ACS Appl. Mater. Interfaces **13** (15), 17869–17881 (2021).

[3]. Bowen Liu, Xiao Su, Yi Lin, Zerui Li, Lingpeng Yan, Yunfei Han, Qun Luo, Jin Fang, Shangfeng Yang, Hongwei Tan, and Chang-Qi Ma, "*Simultaneously Achieving Highly Efficient and Stable Polymer:Non-Fullerene Solar Cells Enabled By Molecular Structure Optimization and Surface Passivation*" Adv. Sci. **9** (7), 2104588 (2022).

O 3.8

Triplet excitons and associated efficiency-limiting pathways in organic photovoltaics based on non-fullerene acceptors

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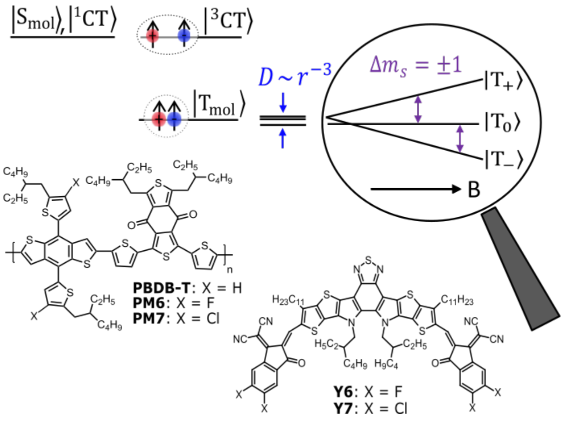

Identifying molecular triplet excitons in state-of-the-art organic photovoltaic

The great progress in organic photovoltaic (OPV) over the past few years has been largely achieved by the development of non-fullerene acceptors (NFAs). However, the power conversion efficiencies are plateauing just below 20%, which rises the importance of identifying and minimizing loss mechanisms. Triplet states are known to adversely affect device performance, since they can form energetically trapped excitons on low-lying states that are responsible for non-radiative losses or even device degradation. Halogenation of OPV materials has long been employed to tailor energy level alignment, morphology and overall enhance device performance. Yet, the influence on recombination to triplet excitons and the possible triplet pathways in advanced OPV materials has not received much attention. Here, the complementary spin-sensitive methods of photoluminescence detected magnetic resonance (PLDMR) and transient electron paramagnetic resonance (trEPR), corroborated by transient absorption (TA) spectroscopy, are applied to unravel exciton pathways in OPV blends, including geminate and non-geminate recombination. Leveraging the strengths of magnetic resonance and optical spectroscopy thereby obtains a complete picture of triplet-formation pathways in state-of-the art OPV blends, employing the polymer donors PBDB-T, PM6 and PM7 together with NFAs Y6 and Y7 [1][2]. All blends reveal triplet excitons on the NFA populated via non-geminate hole back transfer and, in blends with halogenated donors, also by spin-orbit coupling driven intersystem crossing. Identifying these triplet formation pathways in all tested donor:acceptor combinations highlights the untapped potential for improved charge generation to further increase plateauing OPV efficiencies.

References

[1] J. Grüne, G. Londi, A. J. Gillett, B. Stähly, S. Lulei, M. Kotova, Y. Olivier, V. Dyakonov and A. Sperlich, "Triplet Excitons and Associated Efficiency-Limiting Pathways in Organic Solar Cell Blends Based on (Non-) Halogenated PBDB-T and Y-Series" Adv. Funct. Mater. 33, 2212640 (2023).

[2] A. Privitera, J. Grüne, A. Karki, W. K. Myers, V. Dyakonov, T.-Q. Nguyen, M.K. Riede, R. H. Friend, A. Sperlich and A. J. Gillett "Geminate and Nongeminate Pathways for Triplet Exciton Formation in Organic Solar Cells" Adv. Energy Mater. 12, 2103944 (2022).

O 3.9

Transparent Conductive Films of PEDOT:PSS-Amino Acid Composite

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Transparent conductive electrode is an important component of optoelectronic devices such as light emitting diodes, photodiodes, and photovoltaic cells as well touchscreen technology. Growing demand for these technologies, as well as need for functionalities such as cost-effectiveness and flexibility, has resulted in various research on developing organic polymer-based transparent electrodes as an alternative to indium tin oxide (ITO) which is the current industry standard. One of the organic conducting polymers most commonly studied for their potential to be used as ITO-free transparent electrodes is PEDOT:PSS due to its high transmittance as a thin film, solution processability, flexibility, environmental stability, and commercial availability. There have been various works carried out to improve the conductivity of the PEDOT:PSS-based thin films by introducing dopants to improve the charge transport. We present our results demonstrating that the conductivity[1] as well as the transmittance of PEDOT-PSS-based films can be significantly improved by the introduction of amino acids such as phenylalanine in the film. We have observed that this enhancement in conductivity and optical transmittance of PEDOT:PSS-phenylalanine composite film is retained even when the amount of amino acid in the composite films is larger than the amount of PEDOT:PSS. We will present our study on the charge transport mechanism on these films based on DC and AC measurements. We will also further present our studies based on Scanning Electron Microscopy (SEM) as well as Scanning Probe Microscopy techniques such as topography imaging and conducting probe atomic force microscopy (CP-AFM) to elucidate the relationship between film morphology and charge transport in these composite films. The use of bioderived materials such as amino acids to create transparent composite films could open up avenues for developing and integrating bio-based materials in future electronics, help improve the environmental footprint of the electronics, and potentially also allow for the development of materials with a higher degree of biocompatibility for their application in bioelectronics.

References

[1] D. Chamria, C. Alpha, and R. Y. Adhikari, “Phenylalanine-Assisted Conductivity Enhancement in PEDOT:PSS Films,” *ACS Omega*, vol. 8, no. 8, pp. 7791–7799, Feb. 2023, doi: 10.1021/acsomega.2c07501.

Terahertz Spectroscopy as a Tool to Study Charge Carriers in Functional Organic Semiconductors

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Doping of organic semiconductor films enhances their conductivity for applications in organic electronics, thermoelectrics and bioelectronics (Fig. 1). However, much remains to be learnt about the properties of the conductive charges in order to optimize the design of the materials. Electrochemical doping is not only the fundamental mechanism in organic electrochemical transistors (OECTs), used in biomedical sensors, but it also represents an ideal playground for fundamental studies. Benefits of investigating doping mechanisms via electrochemistry include controllable doping levels, reversibility and high achievable carrier densities. We introduced here a new technique, applying in-situ terahertz (THz) spectroscopy directly to an electrochemically doped polymer in combination with time-resolved spectro-electrochemistry and chronoamperometry. We evaluate the intrinsic short-range transport properties of the polymer (without the effects of long-range disorder, grain boundaries and contacts), while precisely tuning the doping level via the applied oxidation voltage. These findings are compared to the THz conductivity of chemically doped polymers (with different processing conditions) and of photoinduced carriers in bulk heterojunction solar cells.

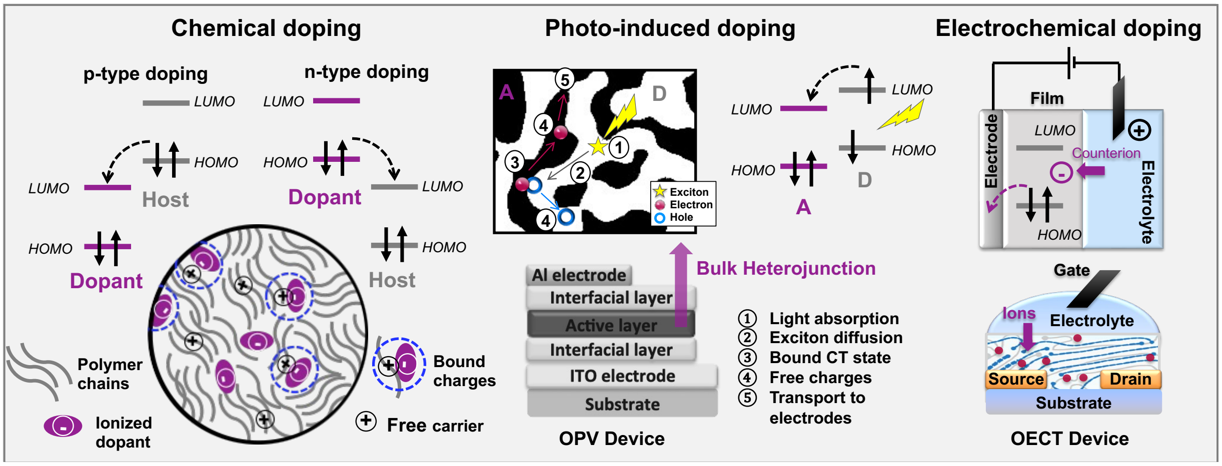

Fig. 1 Charge transfer reactions relevant to the different doping processes that will be investigated in the proposed project, and applications in organic photovoltaic (OPV) and organic electrochemical transistor (OECT) devices.

O 4.2

Probing the electronic and structural properties of organic flexible thin films by in situ spectroelectrochemistry

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Electronically conducting polymers (ECPs) have drawn considerable attention because of their economic importance, good environmental stability, and electrical conductivity. In addition, mechanical, optical, and electronic properties bring versatility for future electronic applications. Many synthetic strategies have been adapted for their preparation, including oxidative chemical synthesis, electrochemical polymerisation and vapour phase polymerisation (VPP). Charge hopping in ECPs with nondegenerate ground state occurs through generated electronic energy levels between valance and conduction band via formation of polaronic states (polarons, polaron pairs/bipolarons, radical cations/dications). These additional energy states formed upon doping and simultaneous charge compensation by dopant ions are accompanied by conformational changes in the polymer network. Such structural, morphological, and optical changes occurring in ECPs during doping-dedoping can be studied using different microscopic and spectroscopic methods. In this work, a fast and easy VPP technique at atmospheric pressure and electrochemical polymerisation has been utilised for the production of conducting poly(3,4-ethylenedioxythiophene) (PEDOT) and polyazulene (PAz) thin films [1, 2]. As a low bandgap material, PEDOT enables reversible electrochemical p- and n-doping and has been used in versatile fields of application. PAz possesses high intrinsic pseudocapacitance, making it a good material for supercapacitor applications. Preferred morphologies and structures with selective dopant ions can be obtained by using and modifying various synthesis parameters and techniques. The in situ Attenuated Total Reflection Fourier Transform Infrared (FTIR-ATR) and UV-Vis spectroelectrochemical techniques were used to probe the influence of polymerisation technique on the structure and the electronic properties and charge carrier formation during n- and p-doping of PEDOT and PAz.

References

[1] R. Yewale, P. Damlin, M. Salomäki and C. Kvarnström, *Layer-by-layer approach to engineer and control conductivity of atmospheric pressure vapor phase polymerized PEDOT thin films,* Materials Today Communications **25**, 101398 (2020)

[2] R. Yewale, P. Damlin, M. Suominen and C. Kvarnström, *Fabrication of electroactive multi-layered polyazulene thin films by atmospheric pressure-vapor phase polymerization,* Materials Chemistry and Physics **275**, 125292 (2022)

O 4.3

Shell effects in electromigrated Cu-nanocontacts under ambient conditions

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Electromigration is an important aspect to consider when metallic nanocontacts are designed. As the nanocontacts to computer functional units shrink in size exponentially following Moore's law, electromigration needs to be considered at a new level [1,2]. In addition, electromigration can be used to fabricate nanocontacts with small contact spaces conveniently [2]. The metals in the electromigrated nanocontact have interesting physical properties even before molecules are inserted in the contact [3]. Here, we show that such metals have electronic states similar to the ones we know from shells in metallic clusters [1]. These shells strongly influence the electronic transport in the nanocontacts and are present even at ambient conditions in the presence of oxidation. The periodicities we observe show that the electrons have a free-electron character and are influenced by triangular orbits.

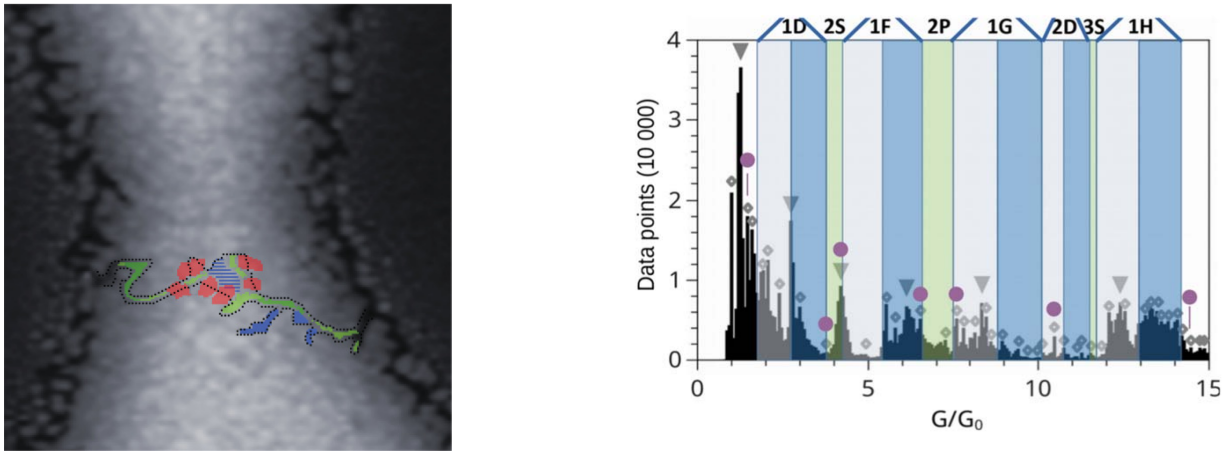

Fig. 1: a) AFM Image of an electromigrated Au nanocontact on SiOx. The area changed by the electromigration has been marked in color [4]. b) Shell effects observed in the histogram of electromigrated Cu nanocontacts observed at ambient conditions in the presence of oxidation [1].

References

[1] J. Hauser et al, "S*hell effects and free-electrons in electromigrated oxidized Cu-nanocontacts*", 2023 Nanotechnology **34**, 175703.

[2] R. Hoffmann-Vogel, "*Electromigration and the structure of metallic nanocontacts*", 2017 Appl. Phys. Rev. **4** 031302.

[3] D. Arnold, M. Marz, S. Schneider and R. Hoffmann-Vogel, "*Structure and local charging of electromigrated Au nanocontacts*", 2017 Nanotechnology **28**, 055206.

O 4.4

Choline ion gel based organic electrochecmical transistors for bioelectronics

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Biocompatible, biodegradable, and solid-state electrolyte-based organic electrochemical transistors are demonstrated. As the electrolyte is composed of all edible-level materials, which are levan polysaccharide and choline-based ionic liquid, the organic transistor fabricated on the electrolyte can be biocompatible and biodegrable. [1] Compared to the other ion gel based electrolytes, it has superior electrical and mechanical properties, large specific capacitance (≈40 μF cm^{-2}), non-volatility, flexibility, and high transparency. Thus, it shows mechanical reliability by maintaining electrical performances under up to 1.11% of effective bending strain, 5% of stretching, and have low operation voltage range when it is utilized in organic transistors. Moreover, the biodegradable electrolyte-based organic transistors can be applied to bio-integrated devices, such as electrocardiogram (ECG) recordings on human skin and the heart of a rat. Moreover, the ionic liquid with PEDOT:PSS allows to change interface orientation.[2] We sincerely analyze the effect of the liquid ions. Based on the materials we developed advanced bioelectronics. The measured ECG signals from the transistors, compared to signals from electrode-based sensors, has a superior signal-to-noise ratio. [3] The biocompatible and biodegradable materials and devices can contribute to the development of many bioelectronics.

Reference

[1] Y.J. Jo, H. Kim, J. Ok, Y.-J. Shin, J.H Shin, T.H. Kim, Y. Jung and Tae-il Kim*****, "Biocompatible and Biodegradable Organic Transistors using a Solid-State Electrolyte incorporated with Choline based Ionic Liquid and Polysaccharide" ***Adv. Funct. Mater.*** 30 (29) 1909707 (2020)

[2] Y.J. Jo, et. al, Unpublished

[3] Young Jin Jo, J. Ok, S.Y. Kim, and Tae-il Kim*, "Stretchable and Soft Organic-Ionic Devices for Body-Integrated Electronic Systems" ***Adv. Mater. Technol.*** 7 (2), 200123 (2022)

O 4.5

Investigate the Effect of Solvent and Additive in Formation of All-Polymer Solar Cells with Situ Optical Spectroscopy

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The morphology of bulk heterojunction (BHJ) is a key factor determining the PV performance and stability of organic solar cells (OSCs). There are many factors determine the morphology of BHJs from liquids to solid films. Here, we investigated the effect of solvent additive and solvents on the formation of all-polymer BHJs with a home-made in -situ Optical Spectroscopy.

Chloronaphthalene (CN) is a common solvent additive employed in OSCs. However, its function has been rarely investigated. We examined the role of CN in all-polymer SCs with in-situ spectroscopies and ex-situ characterization of blade-coated PBDB-T:PF5-Y5 blends. Our results suggest that CN promotes self-aggregation of polymer donor PBDB-T during drying of the blend films, resulting in enhanced crystallinity and hole mobility, which contribute to the increased fill factor and improved performance of PBDB-T:PF5-Y5 OSCs.[1]

Furthermore, we studied the impact of organic solvents on the performance of polymer SCs by investigating the correlation between morphology evolution, charge carrier dynamics and photovoltaic performance by tracking the solution-to-solid transition process of blend films from organic solvent chlorobenzene (CB) and ortho-xylene (o-XY). The drying of PBDBT:PF5–Y5 blends is monitored by in situ multifunctional spectroscopy and the final film morphology is characterized with ex situ techniques. Finer-mixed donor/acceptor nanostructures are obtained in CB-cast film than that in o-XY-cast ones, corresponding to more efficient charge generation in the OSCs. More importantly, the conformation of polymers in solution determines the overall film morphology and the device performance. The relatively more ordered structure in CB-cast films is beneficial for charge transport and reduced nonradiative energy loss. Therefore, to achieve high-performance all-PSCs with small energy loss, it is crucial to gain favorable aggregation in the initial stage in solutions.[2]

Overall, our observations deepen our understanding of the drying dynamics, which may guide further development of all-polymer SCs.

References

[1] Liu Y. et al., “In Situ Optical Spectroscopy Demonstrates the Effect of Solvent Additive in the Formation of All-Polymer Solar Cells,” J. Phys. Chem. Lett. 13, 11696−11702 (2022).
[2] Yao N. et al., “In Situ Study the Dynamics of Blade-Coated All-Polymer Bulk Heterojunction Formation and Impact on Photovoltaic Performance of Solar Cells”, Sol. RRL 2201134 (2023).

O 4.6

A Wearable and Flexible Potentiometric Chloride Activity Sensing Platform with Replaceable Electrodes for Cystic Fibrosis Diagnosis at home

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Potentiometry permits to measure the potential between two electrodes while little to no current passes through the sample, realizing the so-called open circuit potential (OCP) measurement. When ion-selective electrodes (ISE) are used, the measured potential is directly correlated with the ion concentration in the solution, enabling a direct quantitative determination. The ISE consists of the Reference Electrode (RE) and an indicator electrode, commonly identified as Working Electrode (WE), both immersed in the same solution to be analyzed and capable of reacting with it.

This method presents the advantage to make possible the real-time assessment of chloride ion (Cl^-), by measuring the OCP of the ISE with respect to a RE with stable potential, and applying the Nernst equation:

$$E_{OCP} = E_{WE}^{0} + \frac{RT}{nF}\log\left(a_{Cl-}\right) \tag{1}$$

where E_{OCP} is the measured OCP, E_{WE}^0 is the electrode potential for the WE, a_{Cl-} is the activity of the chloride ions near the electrode, R is the gas constant, F is the Faraday constant, and T is the absolute temperature (K). Since the redox reaction Ag ⇔ Ag^++ e^- involves one electron, n=1, the ideal slope of OCP-based sensor is equal to RT/F=59.2 mV per decade of ion activity at room temperature. The OCP-based sensor calibration curve slope must tend to this value determining the sensitivity of the potentiometric sensor.

One of the fields of application of the potentiometry is checking chloride concentration in a fluid [1-3]. Checking for elevated sweat chloride concentration is the key laboratory test to support the diagnosis of Cystic Fibrosis (CF) [1]. Typically, sweat samples are extracted from the patient's arm using a wristband supplied with two electrodes used to entrap pilocarpine (at cathode) into a hydrogel matrix. By applying a small current (iontophoresis), the reagent is forced into the skin inducing sweat. Currently, the sample is analyzed by Medical Laboratories. However, the sweat stimulation and the evaluation require extended waiting periods and sometimes repetitive measurements, rendering them unsuitable for pediatric patients.

In this work, we present the design of a potentiometric chloride activity sensing platform that is wireless, wearable and flexible. The proposed platform serves as a valuable tool for offering initial support to diagnosis of CF and for convenient monitoring of chloride activity within the comfort of own home. The proposed platform is intended to provide real-time support for the diagnosis of CF by gathering and correlating historical clinical data of patients under control. To ensure wearable and comfortable functionalities, a flexible support has been employed for both the multi-working replaceable electrochemical electrodes and the smart electronics. The proposed electronic system embeds a microcontroller, enabling potential reasoning on the acquired data and patient history, while a microchip antenna ensures the wireless transmission of measurements and diagnosis to a remote healthcare center.

References

[1] Gibson L., Cooke R. A test for concentration of electrolytes in sweat in cystic fi-brosis of the pancreas utilizing pilocarpine by iontophoresis. Pediatrics. 1959 Mar;23(3):545-9.
[2] D. De Venuto, M. D. Torre, C. Boero, S. Carrara and G. De Micheli, "A novel multi-working electrode potentiostat for electrochemical detection of metabolites," SENSORS, 2010 IEEE, Waikoloa, HI, USA, 2010, pp. 1572-1577, doi: 10.1109/ICSENS.2010.5690297.
[3] D. De Venuto, E. Stikvoort, D. Tio Castro and Y. Ponomarev, "Ultra low-power 12-bit SAR ADC for RFID applications," 2010 Design, Automation & Test in Europe Confer-ence & Exhibition (DATE 2010), Dresden, Germany, 2010, pp. 1071-1075

O 4.7

Molecular Donor-Acceptor Dyads and Triads for Single Material Organic Solar Cells

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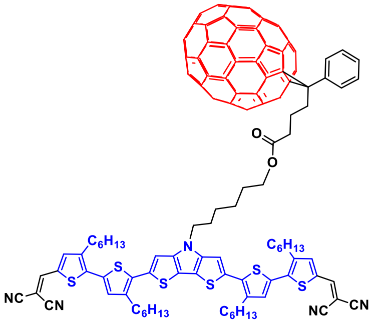
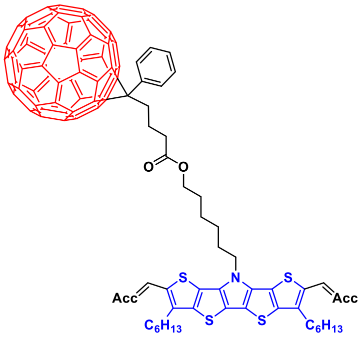
Single material organic solar cells (SMOSC) currently undergo a “renaissance”, because in recent time the photoactive molecules and materials and at once the control of the nanomorpholgy of the photoactive layer have been vastly improved. Facilitated cell fabrication by deposition of only one photoactive component and significantly enhanced reproducibility and excellent stabilization of the microstructure lead to high thermal and light long-term stability as required for industrial applications.[1]

Structurally defined molecular donor (D)-acceptor (A) dyads and triads allow for valuable structure-property relationships and already achieved power conversion efficiencies (PCE) of >5%.[2]

In this respect, we now present our rational molecular design for molecular D-A dyads and triads comprising in a first series a π-conjugated dithienopyrrole (DTP)-based oligothiophene donor with appended fullerene acceptors.[3] In a second series, the core in the donor is represented by more planar *S,N*-heteropentacene (SN5’) units.

Purposeful structural variations and their consequences on physical properties and device performance in SMOSCs were elucidated for both series and qualitative structure-property-device performance relationships obtained.[4]





References

[1] Y. He, T. Heumüller, W. Lai, G. Feng, A. Classen, X. Du, C. Liu, W. Li, N. Li, C. J. Brabec, *Adv. Energy Mater.* **2019**, *9*, 1900409.

[2] (a) S. Lucas, J. Kammerer, M. Pfannmöller, R. R. Schröder, Y. He, N. Li, C. J. Brabec, T. Leydecker, P. Samorì, T. Marzalek, W. Pisula, E. Mena-Osteritz, P. Bäuerle, *RRL Solar* **2021**, *5,* 2000653;
(b) A. Aubele, Y. He, T. Kraus, N. Li, E. Mena-Osteritz, P. Weitz, T. Heumüller, K. Zhang, C. J. Brabec, P. Bäuerle, *Adv. Mater.* **2021**, 202103573.

[3] A. Aubele, T. Kraus, P. Bäuerle, *Chem. Eur. J.* **2023**, submitted.

[4] T. Kraus, A. Aubele, P. Bäuerle, *Org. Chem. Front.* **2023**, accepted.

O 4.8

Photoluminescence properties of single-walled carbon nanotubes modified with Stable Organic Radicals

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Perchlorotriphenyl methyl (PTM) radical is a stable persistent organic free radical with a multifunctional character displaying several interesting properties. This radical is paramagnetic, redox active, fluorescent and chiral. [1,2] PTM radical has been grafted on different surfaces (silicon, gold, ITO, HOPG) via alkene, thiol, silane and and diazonium salt groups, respectively). [3,4] Recently PTM-based surfaces have been investigated as redox-capacitor and paramagnetic switches and molecular wire, among others [3,5,6]. Here, we will present our more recent work on the modification of single-walled carbon nanotubes (SWCNTs) via diazonium chemistry, being this, the first example of SWCNTs covalently modified with PTM radicals.

It is well known that diazonium salts react with SWCNTs generating luminescent *sp*^{3} defects (also called quantum defects or organic color centers), with their characteristic red-shifted emission and long photoluminescence (PL) lifetimes enabling higher PL quantum yields and single-photon emission at room temperature. [7] In this work, the PL studies performed reveal that the presence of the radical leads to partial quenching of the *sp*^{3} defects PL. The mechanism to explain this phenomenon is a combination of a photoinduced electron transfer process and population transfer to triplet states enabled by radical-enhanced intersystem crossing. This result is very promising since it encourages to go deeper in the study of the elusive triplet exciton manifold in carbon nanotubes. [8] Towards this aim, to better understand the mechanism behind, these materials are currently being investigated by Optically Detected Magnetic Resonance (ODMR) which is a technique that combines the spin-sensitive magnetic resonance technique with optical spectroscopy to very sensitively detect triplet excitons in SWCNTs.

Several applications could be envisaged for the herein presented SWCNTs@PTMrad, such the encapsulation of this material into biocompatible surfactants as metal-free contrast agents for magnetic resonance imaging complementary to in vivo near-infrared fluorescence imaging.

References

[1] M. Ballester. Acc. Chem. Res. **18**, 380−387 (1985)
[2] H. Guo et al.; Nat. Mater., **18**, 977–984 (2019)
[3] M. Mas-Torrent et al.; Chem. Rev., **112**, 2506 –2527 (2012)
[4] Gonca Seber et al.; Chem. Eur.J., **23**,1415 –1421 (2017)
[5] Francesc Bejarano et al.; J. Am. Chem. Soc. **140**, 1691–1696 (2018)
[6] J. Alejandro de Sousa et al.; Chem. Sci., **11**, 516 (2020)
[7] Felix J. Berger et al.; ACS Nano, **13**, 8, 9259–926 (2019)
[8] Felix J. Berger et al.; ACS Nano, **15**, 3, 5147–5157(2021)

O 4.9

Optoelectronic properties of two-dimensional organic molecular crystals upon their electronic structure

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Charge transport property of π-conjugated organic semiconductor films is one of key issues in organic electronics, which drives us to pursue novel high-performing molecules and high charge mobility in organic films for efficient optoelectronic devices [1]. However, the soft nature of organic materials induces different molecular packing inside organic solids with variable morphologies, which not only causes inconsistent device performance, but also smears out their intrinsic electronic properties in films. It is urgent to explore organic materials free of structure issues to approach intrinsic properties and stress structure–property relationship, e.g., anisotropic mobility is tightly linked to the molecular arrangement at the interface, as studied in organic field-effect transistors (OFETs), electronic structure in direct relationship with the charge mobility often lacks accurate characterization due to experimental difficulties like small-size crystal sample, charging problem in photoelectron measurements, etc.

The emergence of two-dimensional organic molecular crystals (2DMC) [2] with well controlled thickness provides a great opportunity to explore the structure–property relationship, it can overcome the dimension limitation for device fabrication and electronic study, but also alleviate the sample charging making advanced surface science techniques applicable. Herein, upon successful growth of ~cm^2 size bilayer 2DMCs of C6-DPA on a water surface by the space confined strategy method [3], the film was transferred to variable substrates for device and electronic properties study. The crystal structure of high-quality 2DMCs of C6-DPA were confirmed by multiple characterization techniques, e.g., polarized optical microscopy, transmission electron microscopy with selected-area electron diffraction, x-ray diffraction, atomic force microscopy, angle-dependent near edge x-ray absorption fine structure (NEXAFS), etc. The anisotropic mobility based on OFETs along *b* axis direction is 0.88 cm^2 V^{-1} s^{-1}, while 0.43 cm^2 V^{-1} s^{-1} along *a* axis direction. Furthermore, the valence band feature of 2DMCs of C6-DPA was probed along the surface normal and in *ab* plane by photoelectron spectroscopy with tunable photon energy and angle-resolved ultraviolet photoelectron spectroscopy [5], respectively. The anisotropic valence band dispersion was only observed in the *ab* plane. The in-plane dispersion is clearly along the well-packed [010] direction (*b* axis) and the corresponding effective mass is 3.63m_0 with band-like transport properties. There is no band dispersion direction along [100] (*a* axis). Furthermore, density functional theory calculations were performed to extract the band structure and density of states of the 2DMCs of C6-DPA, which is in line with the experimental results. Our study provides for the first time to correlate between the OFET device performance and electronic properties of the same crystal film, which also paves a way for the perspective studies of 2DMC to shed light on structure-properties relationships of organic materials.

References

[1] S. Fratini, et al., *“Charge transport in high-mobility conjugated polymers and molecular semiconductor”* Nat. Mater. **19**, 491-502 (2020).
[2] H. Jiang, *“The Emergence of Organic Single-Crystal Electronics”* Angew. Chem. Int. Ed. **59**, 1408–1428 (2020).
[3] Q. Wang, et al., *“Space-Confined Strategy toward Large-Area Two-Dimensional Single Crystals of Molecular Materials”* J. Am. Chem. Soc. **140**, 5339-5342 (2018).
[4] Q. Wang, et al *“Anisotropic valence band dispersion of 2D molecular crystals of C6-DPA and its charge transport dependence”* Mater. Adv. **4**, 2201-2206 (2023).
[5] Y. Nakayama, et al., *“Photoelectron spectroscopy on single crystals of organic semiconductors: experimental electronic band structure for optoelectronic properties”* J. Mater. Chem. C **8,** 9090–9132 (2020).

O 4.10

Toroidal Through Space Conjugation in 3D-Aromatic Molecules

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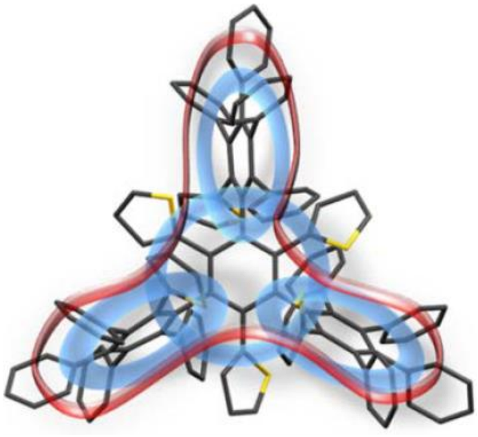
3D polyphenylene and polythienyl dendrimers and nanostructures are not only of great importance due to their wide range of potential applications as nanomaterials, but also attractive for their challenging synthesis and intriguing properties. We have more recently described the development of sterically crowded and twisted thienylene-phenylenes and compared them to their polyphenylene counterparts. Like in the last case, steric hindrance and a propeller-like arrangement of the peripheral thiophene rings are found in the new dendrimers, which opens the way to intriguing properties.

Interestingly, through-space π-conjugation of the ipso-carbons in a toroidal and catenated topology has been evidenced from X-ray structure analysis and extended theoretical calculations including those based on the anisotropy of the induced current density (ACID). Our new synthesized derivatives, which can form stable radical cations or dications, and their physical and electrochemical properties will be shown.



References

[1] A. J. Berresheim, M. Müller and K. Müllen*, Chem. Rev.* **99**, 1747 (1999).
[2] A. Narita, Z. Chen, Q. Chen and K. Müllen*, Chem. Sci.* **10**, 964, (2019).
[3] T. D. Leitner, Y. Gmeinder, F. Röhricht, R. Herges, E. Mena-Osteritz and P. Bäuerle*, Eur. J. Org. Chem.*, 285, (2020).
[4] R. Herges and D. Geuenich*, J. Phys. Chem. A* **105**, 3214, (2001) C. van Trigt, "Visual system-response functions and estimating reflectance," JOSA A **14,** 741-755 (1997).

O 4.11

3D Supramolecular Hybrid Heterostructures on Highly Ordered 2D Thin Film: Coordination Chemistry at Work with Tetrapyrrolic Macrocycles Network

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Photoactive organic-based molecular materials hold a great deal of potentials in many technological and biomedical fields. In this respect, we have undertaken researches exploiting two classes of materials, namely luminescent cyclometalated Iridium complexes[1,2] and tetrapyrrole macrocycles (Fig.1).[3-5] In particular, porphyrins and their constitutional isomers porphycenes are a unique class of molecular materials which can serve as multipurpose scaffolds. They have two H atoms in the inner cavity which are subject to fast tautomerism while, as tetradentate ligands, they can also host almost all the metal ions. Being chemically and thermally stable, their periphery (*meso* and β positions) can be functionalized and engineered for specific scopes and applications. Noticing, on various surfaces they arrange as ordered 2D layer with little defects.

Herein it will be presented how a coherent 2D + n (n = 4), layered heterorganic film is epitaxially grown on an archetypal Fe metal electrode.[5] The ground-breaking achievement is the result of the in-vacuum integration of: chemical decoupling of the basal organic layer (ZnTPP) from the electrode, commensurate 2D-ordering of the ZnTPP film, stoichiometric and orthogonally arranged, molecule-to-molecule coupling between ZnTPP and a di-topic linear bridging ligand (i.e., DPNDI) guided by coordination chemistry. Next we will show the first studies on H2Po continuous and compact 2D/3D vacuum deposited thin films characterized by means of UV-Vis-NIR optical spectroscopies (absorption, emission, surface differential reflectivity-SDR and reflectance anisotropy spectroscopy-RAS) and surface microscopies (i.e. AFM).[3,4] We demonstrate a spectacular reversible chromatic change when the film is exposed to acid.

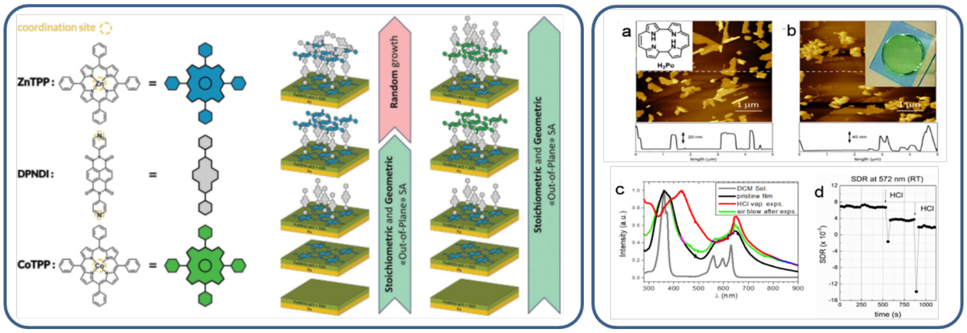

Figure 1. *Left box*, molecular structures of ZnTPP and DPNDI and CoTPP together with their simplified drawings and the obtained molecular construction; *right box*, topography of a) pristine and b) after HCl exposure of H2Po film (inset, green area, film exposed to acid vapors; blue one, unexposed film; c) comparative UV-Vis; d) Surface Diffuse Reflectance (SDR) signals modulation toward HCl vapors exposure.

References

[1] M. Penconi et al. "Advancing Near-Infrared Phosphorescence…" Chem. Mater. **34,** 574−583 (2022)
[2] S. Kesarkar et al. "Near-IR Emitting Iridium(III) Complexes.." Angew. Chem. Int. Ed. **55(8)**, 2714−2718 (2016)
[3] A. Bossi, et al. "Porphycene protonation: a fast and reversible reaction.." ChemPhotoChem **4**, 5264 (2020)
[4] M. Penconi, et al. "Porphycene Films Grown on Highly Oriented Pyrolytic Graphite" Proceedings **56(1)**, 44 (2020).
[5] A. Orbelli Biroli et al., "Out-Of-Plane Metal Coordination for a True Solvent-Free Building with Molecular Bricks…", Adv. Funct. Mater. **31**, 2011008 (2021).

O 4.12

Fast and Accurate Determination of the Singlet–Triplet Gap in Donor–Acceptor and Multiresonance TADF Molecules by Using Hole–Hole Tamm–Dancoff Approximated Density Functional Theory

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One of the requirements to design efficient emitters based on the multi-resonance (MR)- or donor–acceptor (D-A) thermally activated delayed fluorescence (TADF) materials is a relatively small energy gap between the lowest singlet and triplet excited states (ΔE_{ST}). High-level ab initio calculations of their ΔE_{ST} provide benchmark results, but they are very time-consuming and little practical for large-size systems. Here, the performances of the hole–hole Tamm–Dancoff approximated density functional theory (hh-TDA-DFT) and the functional dependent accuracy of hh-TDA are examined on ΔE_{ST} of a large number of MR- and D-A TADF molecules. The results indicate that hh-TDA combined with the hybrid functional B3LYP can predict ΔE_{ST} values for a wide number of MR-TADF molecules with mean absolute error (MAE) within 0.04 eV with correlation as high as 0.75. For D-A TADF molecules, ΔE_{ST} is less sensitive to the nature of the functionals, with MAE as low as 0.07 eV. The larger discrepancy between ΔE_{ST} obtained from hh-TDA-DFT and experimental data in several oxygen-containing MR-TADF molecules is assumed to stem from the aggregation tendency of these compounds in solution. These findings provide important insights into the role of aggregation in reducing the ΔE_{ST} of MR-TADF compounds.

O 4.13

Rationalisation of the Electromechanical Response of an Organic Crystal Assisted by Machine Learning

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In this contribution we present a computational study of the effect of mechanical perturbations on the electronic properties of an organic semiconducting crystal. The chosen molecule, C10-DNBDT-NW, is a well-known high hole mobility material used in organic field-effect transistors (OFET), which was experimentally shown to undergo an increase in its transport properties upon bending of the crystal [1].

We ran a set of classical Molecular Dynamics (MD) trajectories, exploiting ad hoc parameterised force fields, varying the size of the simulation box along two crystallographic axes, so as to simulate the effect of compression and stretching of the crystal. Along each of these MD runs we computed, at DFT level, the values of the hole transfer integral for two pairs of molecules in the middle of the box, corresponding to the two possible transport paths.

We used this set of several thousands DFT calculations to train a Machine Learning (ML) model, with the objective to quickly evaluate hole transfer integrals from an appropriate representation of a dimer. The trained model is able to compute transfer integrals with an error of ~5 meV, well below the typical fluctuations of transfer integrals along an MD trajectory. Thanks to the trained ML model, we proceeded to compute hole transfer integrals between all possible pairs of first neighbours identified in the simulation box, along each MD trajectory, a task clearly computationally unfeasible using quantum mechanical methods.

The trends of the transfer integrals obtained with the ML model averaged over all possible pairs in the simulation box as a function of mechanical strain agree with expectations (*i.e.* higher transfer integrals with compression, lower with stretching), and allow for additional analyses. For instance, the network of couplings computed with the ML model can be used to represent the crystal within graph theory framework, enabling the computation of graph parameters that correlate with transport properties [2]. Visual analyses of the networks as a function of strain show how the transport mechanism shifts from the primary axis to the secondary axis upon stretching of the crystal. The availability of all possible transfer integrals in the simulation box allows computing an average spectral density [3], another computationally cumbersome task if resorting to quantum mechanical methods, which can shed light on the molecular motions coupled with variations of the transfer integrals, to engineer new materials with better transport properties. Finally, it enables to compute the hole mobility within a Kinetic Monte Carlo (KMC) scheme, obtaining a reasonable agreement with experimental measurements.

References

[1] Kubo et al, Nat. Commun. **7**, 11156 (2016).

[2] Jackson et al, J. Phys. Chem. Lett **6**, 1018 (2015)

O 4.14

Simulation of organic mixed ionic and electronic conductors with a combined classical and quantum mechanical model

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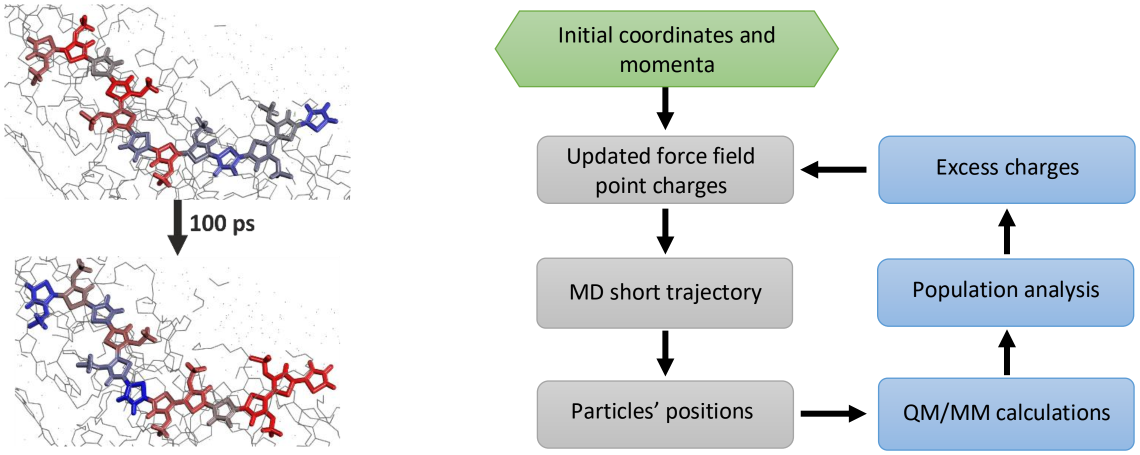
Organic materials that efficiently couple electronic and ionic charge transport (OMIEC) have been recognized as essential in a wide range of technologies [1], from energy storage and generation [2] to nanomedicine and healthcare [3], thanks to their ease of processing, flexibility, low cost, and because they can be finely tuned, e.g. to ensure perfect integration with cellular tissues for nanomedicine or a light weight for energy storage.

Theoretical predictions could represent a great help in developing new materials, tailored for any given application. However, they face the fundamental obstacle that, in these systems, the excess charge is very mobile, and the dynamics of the polymer chain cannot be accurately described with a model including only fixed point charges. Ions and polymer are comparatively slower and a methodology to capture the correlated motions of excess charge and ions is currently unavailable. Considering a prototypical interface for an archetypal OMIEC (poly-thiophene with glycol side chains), we constructed a scheme based on the combination of MD and QM/MM to evaluate the classical dynamics of polymer, water and ions, while allowing the excess charge of the polymer chains to rearrange following the external electrostatic potential [4]. We find that the location of the excess charge varies substantially between chains. The excess charge changes across multiple timescales, as a result of fast structural fluctuations and slow rearrangement of the polymeric chains. Our results indicate that such effects are likely important to describe the phenomenology of OMIEC, and we are working on the introduction of additional features in the model to enable the study of processes such as electrochemical doping.



Left panel: Pictorial representation of charge redistributions in an OMIEC during the dynamics. Right panel: QM (blue)/MD (grey) workflow applied in our study.

References

[1] Paulsen, B. D.; et al. *Nat. Mater.*, **19**, 13 (2019); Chung, J.; et al. *ACS Macro Lett.*, **9**, 646 (2020)
[2] Moia, D.; et al., *Energy Environm. Sci.*, 12, 1349 (2019); Liang, Y.; et al. *Adv. Energy Mater.*, **2**, 742 (2012)
[3] Van de Burgt, Y.; et al. *Nat. Mater.*, **16**, 414 (2017); Giovannitti, A.; et al. *Adv. Mater.*, **32**, 1908047 (2020)
[4] Landi, A.; et al *J. Mater. Chem. C* https://doi.org/10.1039/D2TC05103F (2023)

O 4.15

Organic Electronics from Structural Database: New High Mobility Materials and Design Strategies

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We have used a large database of 40,000 known molecular semiconductors, extracted from the Cambridge Structural Database (CSD), to answer some of the most challenging questions in the field of organic electronics [1]. For instance, we have realized the plausible physical limit to the charge carrier mobility achievable within this materials class [2]. Our detailed investigations revealed that the best-known materials are not ideal with respect to all properties. It is also found that the key properties related to the charge transport are either uncorrelated or "constructively" correlated concluding that a tenfold increase in mobility is within reach in a statistical sense, on the basis of the available data.

The same set of data was also used to answer "how to reduce the dynamic disorder?" [3]. Dynamic disorder is one of the important parameters limiting the charge carrier transport in molecular semiconductors and a parameter that cannot be easily controlled through known design rules. We evaluated the dependence of dynamic disorder on a large number of molecular and crystal characteristics. Our results revealed that the strength of dynamic disorder is highly correlated with the gradient of the transfer integral, a property easily computable for any molecular orientation. We also show that molecular pairs arranged in a "head-to-tail" fashion are more likely to yield low dynamic disorder. This observation is highly counterintuitive as for years the focus has been to maximize the number of pi-stacked atoms. The findings of this work provide important design principles for low-disorder high-mobility molecular semiconductors [3] and open ways for opportunities which have never been explored in molecular semiconductors [4].

References

[1] D. Padula, Ö. H. Omar, T. Nematiaram, A. Troisi, Energy Environ. Sci. **12**, 2412 (2019).
[2] T. Nematiaram, D. Padula, A. Landi, A. Troisi, Adv. Funct. Mater. **30**, 2001906 (2020).
[3] T. Nematiaram, A. Troisi, Mater. Horizons **7**, 2922 (2020).
[4] T. Nematiaram, A. Troisi, Chem. Mater. **33**, 3368 (2022).

O 4.16

Integrated simulation of organic materials: From stationary to dynamical

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Molecules are promising from many aspects ranging from electronics to quantum technology [1,2]. We have modelled the magnetic and optical properties for organic molecules from a wide range of perspectives, including organic electronics, light-emitting diodes, and quantum technology. We are interested in optical properties, opto-spintronics, and quantum computing in organic molecules. For stationary molecular properties, we have recently computed the adhesive energies for P3HT-PVP [3] interfaces and optical properties for DMAC-type molecules [4], by using hybrid-exchange density-functional theory. We have also combined density-functional theory calculations with tight-binding methods to model the ultraviolet-visible optical absorption spectra of molecular chains [5]. Moreover, we have also used first principles calculations and theory of open quantum systems to model the spin dynamics of organic radicals to assess the potential of organic molecules for quantum computing [6,7]. A design of quantum circuit architecture based on integration of molecular network and nano-photonic devices has also been proposed, which not only has potential to raise the number of quantum bits but also to raise the working temperature for quantum computer. Our calculations show that the integration of first principles calculations and dynamics simulations is a powerful tool for the design of organic molecules for different applications, especially quantum computing where dynamical processes are important.

References

[1] P. Friederich, et al, "Toward Design of Novel Materials for Organic Electronics", Adv. Mat. 2019, 31, 1808256.
[2] M. Wasielewski, et al, "Exploiting Chemistry and Molecular Systems for Quantum Information Processing", Nat. Rev. Chem. 4, 490 (2021).
[3] X. Du, et al, "The adhesive energies between P3HT and PVP for organic electronic devices: Hybrid-exchange density-functional-theory studies", J. Phys. Org. Chem., 36, e4494 (2023).
[4] Y. Wang, et al., "The optical spectra of DMAC-based molecules for organic light-emitting diodes: Hybrid-exchange density functional theory study", J. Phys. Org. Chem., e4386 (2022).
[5] Q. Chen, et al., "Optoelectronic properties of one-dimensional molecular chains simulated by a tight-binding model", AIP Advances, 11, 015127 (2021).
[6] L. Ma, et al., "Triplet-radical spin entanglement: potential of molecular materials for high-temperature quantum information processing", NPG Asia Materials, 14, 45 (2022).
[7] J. Chang, et al., "Blueprint of optically addressable molecular network for quantum circuit architecture", arXiv: 2209.04835 (2022).
[8] W. Wu, "A quantum circuit architecture based on the integration of nanophotonic devices and two-dimensional molecular network", SPIE Proceeding, 12335, 139 (2023

O 4.17

High-throughput modelling of semiconducting polymers: a revolutionary route to in silico design of conjugated polymer

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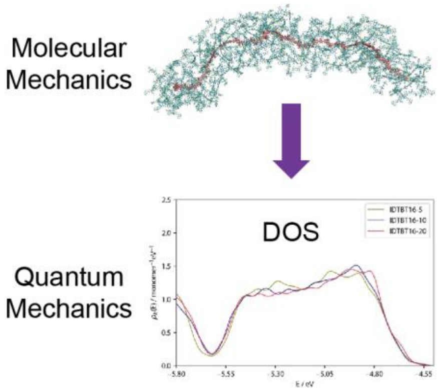
Background. Semiconducting polymers (SCPs) have a wide range of applications due to their ability to be used in low-cost, lightweight, and large-scale electronic devices. The physical properties of SCPs can be tailored by selecting a sequence of conjugated monomers and flexible side chains, which defines the chemistry. So far, materials development in the field has progressed largely by trial and error and **a generic approach that provides the necessary design principles for the desired properties in SCPs is in extremely high demand**. Existing computational methods are used to model SCPs, but there are several challenges that have inhibited the expected progress in the field thus far. Generating atomistic models through conventional MD approaches is a tedious and laborious task due to the lack of standard protocols in organic electronics. As such, compared to the volume of new materials introduced every year there is a very limited number of SCPs with reliable atomistic models since accurate simulations are reserved for just a few polymers per investigation. Expediting polymer modelling is achieved by changing the current approach in modelling of polymers: **instead of building a model for a material, we build a protocol for a material class**, relying on the current research excellence in the group on (i) development of polymer modelling schemes [1], and (ii) high-throughput analysis of organic electronic materials [2]**.**

Objectives of research. We have developed a software package to generate a library of (tens of) existing and hypothetical SCPs by expediting model generation through developing a standard automated workflow. This software: i) employs a multiscale resolution method (from sub-atomic to meso-scale), ii) enables speedy model generation, iii) develops a high-throughput QM/MM method to establish (currently lacking) structure-property relationship database for this material class, and iv) generates new design rules for material development for this material class. In the next step, the generation of hundreds of SCP models will be considered, and it will provide a homogeneous database to enable data science (for the first time) to contribute to materials development in this field.



Results. The calculated (morphological and electronic structure) properties for several (well-studied) modeled polymers (e.g., IDTBT, DPPDTT) are verified against experimental data. Then, the modelled hypothetical SCP structures and their expected properties are analyzed. Furthermore, the high-throughput QM/MM workflow and its performance will be discussed in detail.

References

[1] Seyyed Mohammad Mousavifard, Hassan Ghermezcheshme, Alireza Mirzaalipour, Mohsen Mohseni, Gijsbertus de With and **Hesam Makki**," PolySMart: a general coarse-grained molecular dynamics polymerization scheme"' Mater. Horiz. **2023**, Advance Article.
[2] Tahereh Nematiaram, Daniele Padula, Alessandro Landi, and **Alessandro Troisi**, "On the Largest Possible Mobility of Molecular Semiconductors and How to Achieve It" Adv. Funct. Mater. **2020**, 30, 2001906.

O 4.18

An *ab initio* method on predicting absorption spectra of crystalline organic semiconducting films

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Theoretical description of electronic excited states of molecular aggregates at an ab initio level is computationally demanding. To reduce the computational cost, we propose a model Hamiltonian (MH) approach that approximates the electronically excited state wavefunction of the molecular aggregate. We benchmark our approach on a thiophene hexamer, as well as calculate the absorption spectra of several crystalline non-fullerene acceptors (NFAs), including Y6 and ITIC, which are known for their high power conversion efficiency in organic solar cells. The method qualitatively predicts the experimentally measured spectral shape, which can be further linked to the molecular arrangement in the unit cell.

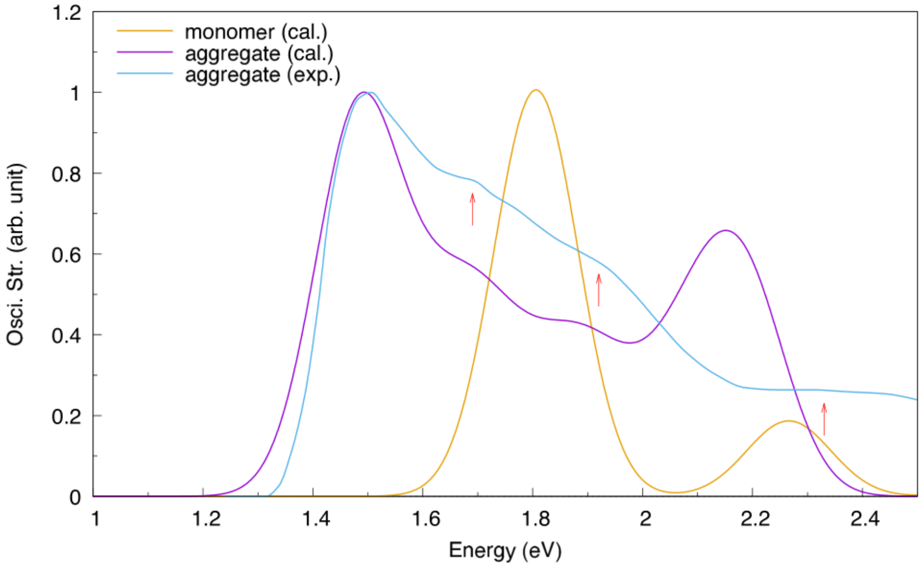

Figure 1: Monomer (orange) and aggregate (purple) as well as the experimental (blue) spectra of the Y6 aggregate.

References

[1] W. Liu, B. Lunkenheimer, V. Settels, B. Engels, R. F. Fink, and A. Köhn, J. Chem. Phys. 143, 084106 (2015)

[2] W. Liu and Denis Andrienko, J. Chem. Phys., 158, 094108 (2023)

O 4.19

Boosting the Fluorescence Yield of a NIR Quantum Emitter

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The figures of merit for single quantum emitters to be applied in quantum photonic applications call – besides single photon purity and indistinguishability – for emission yields close to unity. Considering organic dye molecules, polycyclic aromatic hydrocarbons (PAHs) have shown a number of promising properties for quantum optical applications. A prominent example is the NIR emitter Dibenzoterrylene (DBT) which behaves almost like an electronic two-level system because the probability for intersystem crossing into the long-lived triplet bottleneck state is negligible. Nevertheless, the emission yield of DBT under ambient conditions is far from unity. According to the energy gap law of non-radiative transitions, internal conversion (IC) – non-adiabatic vibronic coupling between S_1 and S_0 - increasingly competes with radiative relaxation with decreasing S_1-S_0 transition energy. Consequently, the fluorescence quantum yields of NIR emitters are typically well below 50 %.

Making use of the unexpectedly strong fluorescence solvatochromism of DBT, we recently have shown the validity of the energy gap law for DBT at the bulk and single molecule level.[1] By controlling the fluorescence lifetime and quantum yield of single DBT molecules, the S_1-S_0 energy gap dictates how these quantities develop during spectral fluctuations (Figure 1).

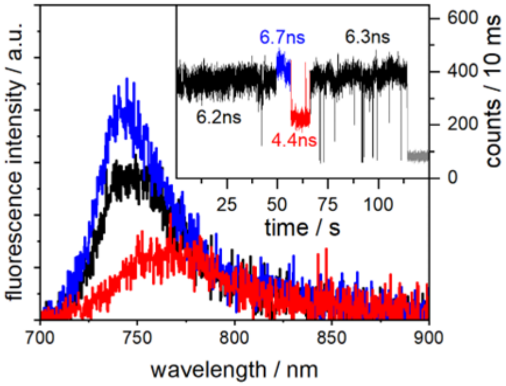

Figure 1: Fluorescence spectra and intensity time trace (inset) of a single (non-deuterated) DBT molecule as a function of time. Fluorescence lifetimes during the different phases are given in the inset.

To model the IC process, it is often assumed that C-H-stretching vibrations serve as accepting modes of the electronic excitation energy. Accordingly, if the IC rate dominates S_1 relaxation, a deuterium isotope effect may be expected. Concerning PAHs, however, distinct experimental demonstrations are more than scarce. We will show at the bulk and single molecule level that partial and full deuteration of DBT leads to an average increase of the fluorescence lifetime and quantum yield of up to 70 %. Occasionally, we find fluorescence lifetimes close to 14 ns for single fully deuterated DBT molecules. Considering a radiative lifetime of ~ 17 ns, deuteration has turned DBT into an exceptionally bright NIR single quantum emitter even at room temperature.

References

[1] C. Erker, Th. Basché, J. Am. Chem. Soc. **144**, 14053-14056 (2022).

O 5.1

Organic Optoelectronic Components in a Smart-integrated System for Plasmonic-based Sensing

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The continuous growth of the global population has been remarking the need of early detection systems to prevent the spread of epidemics as well as to improve the standards of living. The emerging demand of sensing technologies has prompted researchers and industrial companies to develop devices able to monitor medical, food, water, and environmental safety/quality indicators in an efficient, simple, and reliable way. While high sensitivity and selectivity must be guaranteed, compactness, user-friendliness and low-cost are key characteristics to enable the use of the sensing technology for point-of-care diagnostics without the need for trained personnel [1].

Among state-of-the-art methodologies for pollutants detection, optical sensing has emerged as one of the most simple, versatile, and powerful approaches for analytical purposes. However, a major obstacle towards the development of a portable system has been the use of bulky optical components (e.g. lasers and optical fibers), which are necessary to ensure a good sensing capability. In particular, huge interest has been attracted by functionalized metallic surfaces based on surface plasmon resonance (SPR), as extremely sensitive, label-free, quantitative systems for real-time detection of single or multiple analytes. However, the need of a fine and precise control of the angle of the incident light ended up in the use of not-portable optical components in the final sensor [2]. In this scenario, organic optoelectronic components might enable the definition of new miniaturized detection schemes to boost the advent of compact optical sensors for on-site analysis, given their inherent capability of smart monolithic integration in nm-thick multi-stack devices on almost any surface.

Here, we report an unprecedented ultra-compact system endowed with optical and plasmonic sensing capabilities through the smart integration of (i) organic light-sources such as organic light-emitting diodes (OLEDs) or transistors (OLETs), (ii) an organic light-detector such as organic photodiode (OPD) and (iii) a sensing nanostructured surface such a nanoplasmonic grating (NPG) [3]. The components and the layout of integration were suitably designed to make the elements work cooperatively in a reflection-mode configuration. In particular, the OPD was vertically stacked onto the source electrode of the OLET thus providing electrical switching, light-emission and light-sensing capability in a single organic multilayer architecture. When coupled to the NPG, a multifunctional system with SPR-sensing ability was obtained at a remarkably high level of miniaturizationat a sensor size as low as 0.1 cm^3, arising from the direct fabrication of the NPG onto the encapsulating cap of the light-emitting/-sensing platform [4].

Once finalized into a working prototype and operated with standard solutions, the sensor is calibrated by providing quantitative and linear response that reaches a limit of detection of 10^{-4} refractive index units. Analyte-specific and rapid (15 min long) immunoassay-based detection is demonstrated for targets relevant for the milk chain. By using a custom algorithm based on principal-component analysis, a linear dose–response curve is constructed which correlates with a limit of detection as low as 3.7 µg mL^{-1} for lactoferrin, thus assessing that the miniaturized optical biosensor is well-aligned with the chosen reference benchtop SPR method.

[1] R. Dragone, …, S. Toffanin Frontiers in Public Health, 2017, 5, 1.
[2] M. Prosa, ..., S. Toffanin Nanomaterials 2020, 10, 480.
[3] M. Bolognesi, ..., S. Toffanin Adv. Mater. 2023 2208719
[4] M. Prosa, ..., S. Toffanin, Adv Funct Mater 2021, 31, 2104927.

O 5.2

Sustainable manufacturing of reduced-graphene oxide electrolyte-gated transistors: characterization, understanding and applications

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Nowadays, many societal challenges are arising related to environmental sustainability. Within this context, the development of sustainable approaches to fabricating electronic devices is of paramount importance to envision the future electronics that must support our daily actions.

Here, it is presented a green and versatile protocol for manufacturing electrolyte-gated transistors (EGTs) based on reduced graphene oxide (rGO).[1] This protocol fixed two fundamental issues: i) GO adhesion onto rigid (*i.e.* Si) and flexible (*i.e.* PET) substrates and, ii) its spatially-resolved and fast reduction. A multi-methodological investigation (*viz.* SEM, AFM, two-terminals electrical measurement, Raman spectroscopy etc.) corroborated the electronic and morphological features of such rGO thin-film. This led us to fabricate a robust and reproducible EGT capable to be operated in different electrolytes, namely Milli-Q water, NaCl, artificial sweat etc. Furthermore, rGO-based EGT succeeded to operate under mechanical stress as well as a capillary flow of electrolytes driven by paper-based fluidics.

Aiming at sound electronic applications, it has been decided to deepen our understanding of the functioning of these devices, so we exploited a well-known model for disordered organic thin-film transistors together with a parallel resistance. This allowed us to extrapolate rigorously different parameters such as threshold voltage, mobility, mobility enhancement factor, gain etc.[2]

According to this comprehensive knowledge of this device, we decided to fabricate a sensor towards K^+ and Na^+ cations in artificial sweat.[3] Such a sensor showed excellent sensitivity (*viz.* 1uA/pK and 1uA/pNa) and selectivity: the former relies on the electronic features of rGO-based EGT, whereas the latter takes advantage of the unique properties of the ion-selective membranes (ISMs). This sensor succeeded to detect these cations within a range from 10uM to 100mM with a fast response time (<30 seconds).

Finally, we can state that these devices are extremely promising because they represent an outstanding compromise in terms of cost-effective manufacturing, sustainability, versatility and electrical performance.

References

[1] R. De Oliveira, "Liquid-Gated Transistors Based on Reduced Graphene Oxide for Flexible and Wearable Electronics," Adv. Funct. Mater. **1905375** (2019).
[2] N. Lago, "Characterization and Modeling of Reduced-Graphene Oxide Ambipolar Thin-Film Transistors", IEEE Transactions on Electron Devices 69(6), 3192-3198 (2022)
[3] R. De Oliveira, "Selective Ion Sensing in Artificial Sweat Using Low-Cost Reduced Graphene Oxide Liquid-Gated Plastic Transistors" Small **2201861** (2022).

O 5.3

Kelvin-probe force microscopy of surface potential shift triggered by affinity binding in large-area bio-functionalized surfaces

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A few antigen-antibody binding events generate extended and irreversible surface potential changes on large-area biofunctionalized surfaces. This phenomenon is central for electrolyte gated transistor biosensors that have demonstrated single molecule detection capability, selectivity, compactness and robustness of the electronic transduction. [1–3] The electrical signal arises from the integrated response triggered by selective binding events and is amplified by complex collective phenomena generated at the biolayer interface. With the aim of highlighting the chain of collective physical and chemical processes responsible for the huge amplification of the transduction signals we have used a combination of atomic force and Kelvin probe force microscopies. [4] Our results compare well with the electrical characteristics of single-molecule electrolyte-gated transistor sensors and our statistical modeling based on Einstein's diffusion-theory of ligands. [5] Our findings have profound implications for understanding the chain of irreversible and cooperative surface state transitions induced by a ligand/receptor interaction even on physisorbed bioreceptor layers.

References

[1] Macchia, E. et al. Single-molecule detection with a millimetre-sized transistor. Nat. Commun. 9, (2018).
[2] A sensor detects the light touch of a single molecule. Nature 560, 413–413 (2018).
[3] Macchia, E. et al. Large-Area Interfaces for Single-Molecule Label-free Bioelectronic Detection. Chem. Rev. (2022) doi:10.1021/acs.chemrev.1c00290.
[4] Di Franco C. *et al.*, Extended Work Function Shift of Large-Area Biofunctionalized Surfaces Triggered by a Few Single-Molecule Affinity Binding Events, Advanced Materials Interfaces (2022), https://doi.org/10.1002/admi.202201829
[5] Macchia, E, De Caro, L., Torricelli, F., Di Franco, C., Mangiatordi, G.F. Scamarcio, G., Torsi, L, Why a Diffusing Single-Molecule can be Detected in Few Minutes by a Large Capturing Bioelectronic Interface, Advanced Science, (2022) 9, 2104381.

O 5.4

Multiparametric nanocharacterization of electrolyte gated organic transistors in operando

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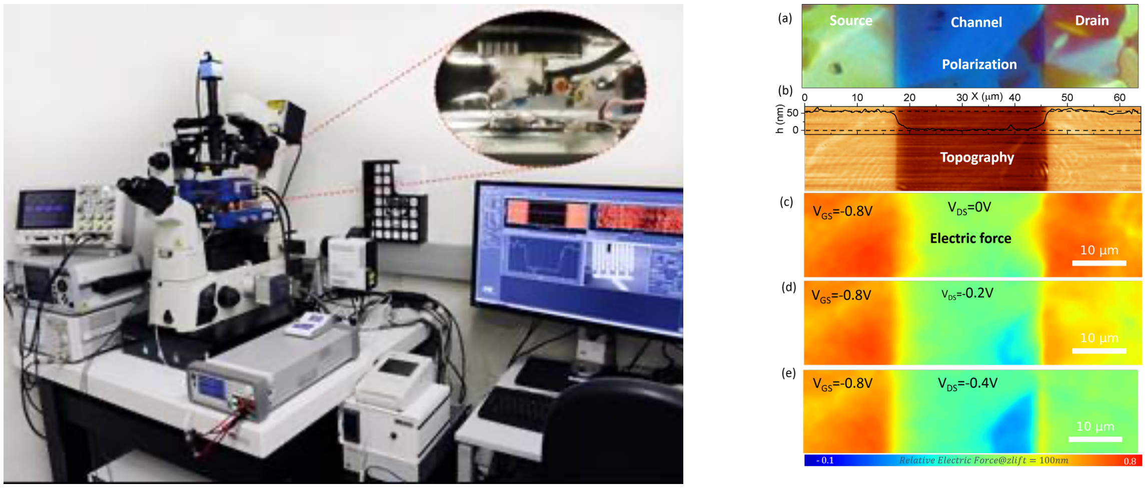
Electrolyte-Gated Transistors (EGTs) have emerged as an integral part of numerous applications in biosensing and bioelectronics, owing to their remarkable ability to efficiently transduce biological events into amplified electronic signals while stably operating in aqueous electrolytes. A typical EGT is a three-terminal device consisting of a semiconducting channel between source and drain electrodes capacitively coupled with the gate electrode through ions in the electrolyte. Understanding these devices at the nanoscale is paramount in order to leverage their respective, or combined, functionality for various applications. An optimized level of crystallinity or a balance between ionic and electronic conduction within the semiconductor might be desired, which directly relates to the physical and chemical nature of the semiconducting material and its response to applied electric fields. However, probing the nanoscale properties under operating conditions has been challenging due to the complications arising from the electrolyte environment.

In this communication, I will review the progress made in our research group towards developing an advanced scanning probe microscopy technique able to probe different functional properties of the semiconductor materials (morphology, electrical, mechanical) at the nanoscale in operating electrolyte-gated transistors (EGTs). The technique is based on in-Liquid Scanning Dielectric Microscopy (in-Liquid SDM) to which we added automated functionalities and multiparametric characterization capabilities for comprehensive and simultaneous probing of the nanoscale electrical, mechanical and morphological properties in operating EGTs. Examples of applications to Electrolyte Gated Organic Field Effect Transistors (EGOFETs) [1], [2] and Organic Electrochemical Transistors (OECTs) will be presented [3].



Left: Multiparametric in-liquid SDM setup for in operando EGTs nanocharacterization. Right: Polarization, topographic and electric force images at different applied voltages of an EGOFET.

[1] Kyndiah, A. et al. Adv. Funct. Mater. **31**, 2008032 (2021).
[2] S. Tanwar et al. (in preparation).
[3] S. Tanwar et al. (in preparation).

O 5.5

Contact Resistance of Low-Voltage n-Channel Thin-Film Transistors Based on Three Different Organic Semiconductors

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Many applications envisioned for organic thin-film transistors (TFTs) are mobile devices for which a low power consumption is one of the most critical requirements. From a circuit-design perspective, the most effective approach to minimize the power consumption is to combine p-channel and n-channel transistors in a complementary design. However, the performance of even the best n-channel organic TFTs still lags behind that of p-channel organic TFTs. Here, we compare the performance of low-voltage n-channel organic TFTs based on three promising small-molecule semiconductors, namely N,N'-bis(2,2,3,3,4,4,4-fluorobutyl)-(1,7 & 1,6)-dicyano-perylene-tetracarboxylic diimide (ActivInk N1100) [1], 2,9-bis(heptafluoropropyl)-4,7,11,14-tetrabromo-1,3,8,10-tetraazaperopyrene (TAPP-Br_4) [2] and diphenylethyl-3,4,9,10-benzo[de]isoquinolino[1,8-gh]quinolinetetracarboxylic diimide (PhC_2-BQQDI) [3]. The TFTs were fabricated on silicon or flexible plastic substrates using a hybrid gate dielectric composed of a thin, plasma-grown aluminum oxide layer and a tetradecylphosphonic acid self-assembled monolayer. We fabricated TFTs both in the staggered (top-contact) and in the coplanar (bottom-contact) device architecture, using gold for the source and drain contacts. In the coplanar TFTs, the surface of the gold source and drain contacts was treated with a chemisorbed interface layer based on one of four different thiols. All electrical measurements were performed in ambient air. For each of the three semiconductors, the TFTs fabricated in the coplanar architecture were found to have a smaller contact resistance than the staggered TFTs. Regardless of the semiconductor, the best TFT performance was obtained by functionalizing the contacts with 4-(methylsulfanyl)-thiophenol (MeSTP). Flexible coplanar TFTs based on the semiconductor PhC_2-BQQDI with MeSTP-functionalized contacts have an intrinsic channel mobility up to 0.8 cm^2/Vs, an on/off current ratio up to 10^6, a subthreshold slope as small as 85 mV/decade, and a contact resistance as small as 210 Ωcm (a record for n-channel organic TFTs).

References

[1] B. A. Jones, “High-mobility air-stable n-type semiconductors with processing versatility: Dicyanoperylene-3,4:9,10-bis(dicarboximides),” Angew. Chem. Int. Ed. **43**, 6363-6366 (2004).

[2] S. Geib, “Core-brominated Tetraazaperopyrenes as n-channel semiconductors for organic complementary circuits on flexible substrates,” Adv. Funct. Mater. **23**, 3866-3874 (2013).

[3] T. Okamoto, “Robust, high-performance n-type organic semiconductor,” Sci. Adv. **6**, eaaz0632 (2020).

O 5.6

Ambipolar transport and space-charge accumulation effects in organic heterojunction field-effect transistors

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In this contribution, we report on the fabrication and characterization of organic heterojunction field-effect transistors based on the combination of various conjugated organic compounds (see the related structures in Fig.1) deposited in form of thin films. The morphological, electrical and electronic properties of devices featuring double-layer, triple-layer and co-deposited (blend) active channels were investigated using a wide number of complementary techniques.

Firstly, field-effect devices were fabricated through the sequential evaporation of picene and PDIF-CN_2 molecules[1]. By exploiting the related different self-assembling properties, with picene showing a dominant 3D growth-mode character, ambipolar transistors, based on double layer active channels and exhibiting balanced hole and electron mobility values both in the range of 0.1 cm^2 / (V ·s), were achieved (Fig.1e). A further enhancement of the final response was obtained by completing the channel with an amorphous PDIF-CN_2 active layer providing a significant effect on the threshold voltage shift.

In a second set of experiments, we analyzed the response of field-effect transistors featuring active channels composed by spin-coated films of P3HT and evaporated overlayers of PDF-CN_2. The electrical characterization demonstrated that the presence of a PDIF-CN_2 film induces a semiconductor-to-conductor transition in the P3HT polymer[2]. The charge doping effect was investigated by Scanning Kelvin Probe Force Microscopy as a function of the PDIF-CN_2 coverage and nominal thickness. Similar charge-transfer effects have been preliminarily observed in a third type of structure based on evaporated C_8-DNTT/PDIF-CN_2 bilayer with the bottom layer showing hole mobility values up to 5 cm^2 / (V ·s).

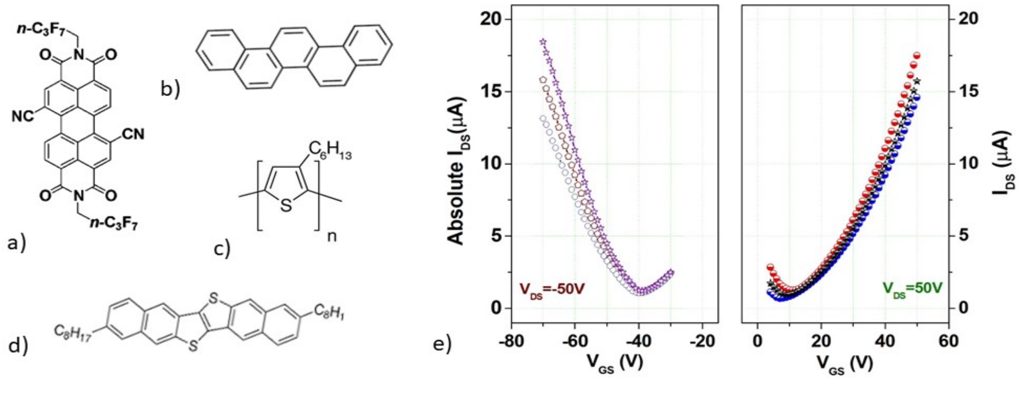

Fig.1 Molecular structures of the investigated compounds: a) PDIF-CN_2, b) picene, c) P3HT, d) C8-DNTT; e) Ambipolar reponse of a picene/PDIF-CN_2 heterojuntion transistor

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References

[1] T. Taguchi, F. Chiarella, M. Barra, F. Chianese, Y. Kubozono, A. Cassinese, Acs Applied Materials and Interfaces, 13 (7), 8631, 2021
[2] F. Chianese, S. Fusco, M. Barra, F. Chiarella, A. Carella A. Cassinese, Journ. of Materials Chemistry C, 9 (47), 17143, 2021

O 5.7

Brewer’s spent grain for greener OTFT structures

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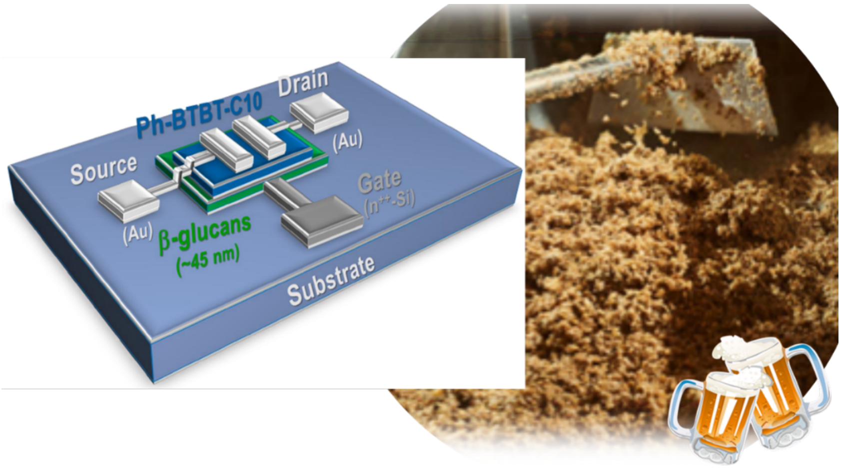
Brewer's spent grain (BSG) represents a major by-product of the brewing industry, accounting for ~85% of the total by-products[1]. The annual global production of BSG is therefore massive, that is ~40 million tons. In the EU, the production is ~ 3,4 million tons. Currently, BSG is mainly sold to farmers (~70% in EU) as low-value animal feed or landfilled (~20%). Finding alternative, higher-value uses for BSG is therefore particularly attractive from the point of view of brewery economics.[1] On the other hand, single-use electronics for smart food and beverage packaging applications require environmentally safe and/or biocompatible devices, with low-cost, and large volumes processability[2]. Therefore, BSG could offer an interesting opportunity to pursue in this context.

In this communication, we present the results of a study on the potential of the inherently biodegradable non-starch polysaccharide components of BSG (i.e., arabinoxylans and mixed linkage (1-3,1-4)-beta-D-glucans) to be employed as a gate dielectric in low-voltage operating organic thin-film transistors (OTFTs). (Figure 1) Note that green solvents were successfully used in OTFT device processing[2].

To further demonstrate the promising possibilities and applications of BSG in a more sustainable organic (opto)electronic technology, we also present the preliminary results on the use of water-soluble arabinoxylans for the realization of transparent and mechanically stable foil substrates for flexible devices.

Fig.1. Left panel: Schematic illustration of a representative BSG-based OTFT device structure. Right panel: Brewers’ spent grain.



Ilary Belardi is grateful PON “Ricerca e Innovazione” 2014-2020, Action IV.5 for funding.

[1] W.G. Sganzerla, L.C. Ampese, S.I. Mussatto, and T. Forster-Carneiro, “A bibliometric analysis on potential uses of brewer’s spent grains in a biorefinery for the circular economy transition of the beer industry”, Biofuels, Bioproducts and Biorefining, 15, 1965–1988 (2021).

[2] A. Marrocchi (Ed) “Sustainable strategies in organic electronics” Woodhead Publishing Series in Electronic and Optical Materials. Elsevier, 2022. ISBN: 9780128231470

O 5.8

Printed Bioelectronics via In-Situ Enzymatic Polymerization of Conjugated Oligomer-based Hydrogel Bioinks

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Hydrogels are an attractive material system for interfacing between medical devices and human neural tissues due to their similar mechanical properties. However, most conventional hydrogel-based bio-interfaces lack electrical conductivity and thereby cannot relay electrical signals related to neural recording and activation. Here we show how *in situ* enzymatic polymerization of the conjugated oligomer-based hydrogel can be utilized to create cell-compatible and electrically conductive hydrogel structures. Conductive hydrogel structures were fabricated using 3D printing of hydrogel bioinks loaded with conjugated oligomers, followed by enzymatic polymerization of the conjugated oligomers by horseradish peroxidase. The polymerization of the conjugated oligomers modified the electroactivity of the hydrogels and resulted in a significant increase in stiffness from about 0.6 kPa to 1.5 kPa. Both the components and polymerization process as well as the resulting conductive hydrogels were well tolerated by both human primary fibroblasts and PC12 cells. This work thus shows possibilities to fabricate cytocompatibility and conductive hydrogels that can be processed using bioprinting. In addition, these hybrid materials show tissue-like mechanical properties, and the hydrogels possess mixed ionic and electronic conductivity, which can provide new means to leverage electricity to manipulate cell behavior in a native-like microenvironment.

References

[1] Strakosas X, Biesmans H, Abrahamsson T, et al. Metabolite-induced in vivo fabrication of substrate-free organic bioelectronics[J]. Science, 2023, 379(6634): 795-802.
[2] Knowlton S, Anand S, Shah T, et al. Bioprinting for neural tissue engineering[J]. Trends in neurosciences, 2018, 41(1): 31-46.

O 5.9

Enhancing the Performance of State-of-Art solar cells by improving the Built-in Potential

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Organic solar cells (OSCs) have attracted great interest in recent years. OSCs based on modern materials achieved great performances as high efficiencies were reported for cells based on non-fullerene acceptors (NFA), however, the efficiency of these devices is still well below its theoretical limit.[1]

The fill factor (FF) of NFAs-based devices is considered a critical limiting parameter to further enhance the cells' efficiency [1]. Photogenerated charge carriers must rapidly be driven away from the junction and be extracted by the electrodes. However, the operating regime of the solar cell is at the maximum power point where the internal field is low. The low extraction rate of charge carriers increases the probability of their recombination before being collected, which results in an overall reduced fill factor (FF) and lower PCE values. Improved FF can be achieved by enhancing the extraction process by the device structure. The above can be done by maximizing the built-in potential and/or enhancing the internal electric field near the junction. [2]

To prove this point, we investigate a bulk-heterojunction device based on PBDB-T-2F (PM6) and Y6 (BTP-4F) as the donor-acceptor pair,[3] respectively. Most reported devices utilize silver as the cathode. The simplest method to enhance the built-in field would be to replace it with Magnesium (Mg). We show that adding a thin layer of Mg below the silver enhances the PCE of the device from 15.8% to 16.8%. Using device modelling of the JV curves, we show that the improved PCE is due to enhanced built-in potential.

Next, based on a previous work done by our group [4] that suggests a new engineering approach using modulation doping to increase the electric field within the cell, we developed a strategy to extend the applicability of the design to modern materials produced through solution processing and make it universal to (almost) any donor-acceptor pair. We suggest a solution-processed universal hole extraction layer (UHEL) structure having a thin doped layer (delta-doping) in its middle. Using cross-linking approach [5], we fabricated the required triple-layer structure. We will first describe the general properties of the enhanced charge-extraction structure and then the complete cell based on PM6: Y6.

References:

[1] Wang, J., Yao, N., Zhang, D., Zheng, Z., Zhou, H., Zhang, F., & Zhang, Y. (2020). Fast Field-Insensitive Charge Extraction Enables High Fill Factors in Polymer Solar Cells. ACS Applied Materials & Interfaces, 12(34), 38460-38469.

[2] Yuan, J., Zhang, Y., Zhou, L., Zhang, G., Yip, H. L., Lau, T. K., ... & Zou, Y. (2019). Single-junction organic solar cell with over 15% efficiency using fused-ring acceptor with electron-deficient core. Joule, 3(4), 1140-1151.

[3] N. Tessler, "The band-gap enhanced photovoltaic structure," Applied Physics Letters, vol. 108, no. 18, p. 183503, 2016.

[4] Shekhar, H., & Tessler, N. (2020). 15% enhancement of the photocurrent at the maximum power point of a thin film solar cell. Sustainable Energy & Fuels, 4(11), 5618-5627.

[5] O. Solomeshch, V. Medvedev, P. R. Mackie, D. Cupertino, A. Razin, and N. Tessler, "Electronic formulations - Photopatterning of luminescent conjugated polymers," Advanced Functional Materials, vol. 16, no. 16, pp. 2095-2102, 2006.

O 5.10

Printed Wearable Electronics for Healthcare

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Additive manufacturing (AM) routes, in particular direct writing (DW) non-contact techniques from liquid precursors (inks) are currently gaining a great deal of interest within the research community and industrial sector, due to the benefits provided in terms of the allowed design freedom, architectural flexibility and industrial scalability. The latter is sustained by relatively small investments and fabrication costs, while guaranteeing the rapid prototyping of desired artifacts. Based on current trends, these technologies have a strong impact in the context of flexible/bendable and conformable electronic devices. They typically require simple manufacturing steps combined with a wide range of printable materials, low cost, reduced waste and fine features. Among DW non-contact techniques, Ink-jet Printing (IJP) and Aerosol Jet Printing (AJP) have been massively employed during the last decade to implement several electronic devices, including biosensors. AJP technology exploits the ink atomization through two processes, i.e. the ultrasonic and the pneumatic atomization, allowing the material deposition over flat and curved substrates [1]. The ability to atomize liquid precursors by two different processes largely increases the range of printable materials (viscosity range between 1 and 1000 cPs), thus exceeding one of the major limitations of IJP techniques.
This contribution shows the use of AJP technique to develop applications in bioelectronics. The first example shows a comprehensive characterization of PEDOT:PSS deposition based on a systematic analysis of the overspray effect, which is aimed at preliminary spotting the proper deposition parameters for minimizing defects and short circuits between near patterns. It is then shown the voltage amplifying capability for small amplitude time-varying signals of a fully printed planar organic transistors, consisting of printed Silver electrodes (source, drain and gate), a PEDOT:PSS active layer deposited using the best deposition parameters from the previous analysis, and a passivation layer for interconnections made of NEA 121, all layers being printed on a flexible Kapton substrate [2]. The second example will report the development of an electrochemical biosensor for the detection in biological fluids of the interleukin 6 (IL-6), a cytokine associated to potential inflammation states. IL-6 detection is based on the antigen-antibody selective binding, including the EDC-NHS chemistry to drive the formation of a self-assembled monolayer (SAM). An ink based on Thermally Exfoliated Graphene Oxide (TEGO) is developed and used to cover the working electrode of a Screen Printed Electrode (SPE). TEGO directly provides a defective surface (i.e. presence of oxygenated species, such as carboxyl and carbonyl groups) available for antibody anchoring, hence avoiding time and cost consuming post deposition processes [3]. Electrochemical Impedance Spectroscopy (EIS) was used to access the detection of IL-6 in real saliva samples, while a measurement protocol involving single SPEs for each IL-6 concentration and providing reproducible measurements, has been adopted to assess a calibration curve showing a Limit of Detection (LoD) falling with in IL-6 physiological range (units of pg/ml).

References

[1] E. Secor, "Principles of aerosol jet printing," Flex. Print. Electron **3,** 035002 (2018).

[2] G. Tarabella, "Aerosol Jet Printing of PEDOT:PSS for large area flexible electronics," Flex. Print. Electron **5,** 014005 (2020).

[3] K. Parate, "Aerosol-Jet-Printed Graphene Immunosensor For Label-Free Cytokine Monitoring in Serum" ACS Appl. Mater. Interfaces 12, 7, 8592-8603 (2020).

Abstracts – short poster presentations

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The recommended poster format is A1 Size (59.4 cm wide x 84.1 cm height). Double-sided adhesive tape and/or pins will be available in the poster area to put the posters on the panels.
Authors are required to print their own poster (printing services will NOT be available on-site) and to take care of putting up their poster before the start of the session and of removing it after the session end.
Each panel will be marked with the number of the poster as identified in the program.
Please place the poster on the correct panel.

POSTER SESSION 1 - October 2nd, 2023 18:00-19:30

P1.1	Hu	Wei-Hsu	Single-Component Squaraine Organic Upconversion Photodetectors with Peak Sensitivity at 1140 nm
P1.2	Kazlauskas	Karolis	Ytterbium Doping of Electron Transport Layer: Impact on Blue TADF-OLED Performance and Stability
P1.3	Ciganek	Martin	Dithioketopyrrolopyrroles (DTPPs) as near-infrared absorbing n-type semiconductors
P1.4	Truksa	Jan	Spectroscopy of Lumazine and Alloxazine in the Binary DMSO-Water Mixture
P1.5	Simotko	Sasha	Understanding the Effects of Processing Conditions on Non-Fullerene-Based Organic PhotodiodePerformances
P1.6	Moscovich	Noam	Blending a Polyelectrolyte with a Mixed Ionic/Electronic Conducting Polymer for OECTs
P1.7	Abelairas	Adrian M.	Preparation of nanographene by iterative organic synthesis
P1.8	Mitoma	Nobuhiko	Graphitic Carbon Nitride Films for Electrical and Optical Applications
P1.9	Hayakawa	Ryoma	Room-Temperature Operation of Vertical Tunnel Transistors with Organic Molecules as Quantum Dots
P1.10	Millan	Judith	Quantum Chemical Calculations on Functionalized DTPs: Stable Components for Organic Semiconducting Materials
P1.11	Spoltore	Donato	Hole transport in low-donor content organic solar cells: the role of the acceptor
P1.12	Vembris	Aivars	Modification of work function of transparent conductive oxides by UV radiation
P1.13	Jain	Nakul	Impact of thermally activated charge separation with offsetnon-fullerene acceptors
P1.14	Grzibovskis	Raitis	Energy level studies of self-assembling monolayer materials using photoelectron emission spectroscopy methods
P1.15	Cordero-Solano	Karla Vanessa	Understanding Contact Resistance In Nanoscale Organic Thin-Film Transistors
P1.16	Gatto	Marco Filippo	Highly-oxidised indolocarbazoles: ideal open-shell candidates for single-molecule electronics
P1.17	Cai	Xinyi	Thermally activated delayed fluorescent organic scintillators for high resolution X-ray imaging
P1.18	Björkström	Kim	Impact of long-term voltage cycling on functionalized thiol-SAM electrodes in EGOFET-based applications
P1.19	Keruckiene	Rasa	Experimental and theoretical study of exciplex-forming compounds containing trifluorobiphenyl and 3,6-di-tert-butylcarbazole units and their performance in OLEDs
P1.20	Vercelli	Barbara	Blue-emitting Carbon Quantum Dots from Hydrothermal Approach: Purification Strategies Comparison and Influence of the Reaction Parameters on the Spectroscopic and
P1.21	Lee	Jae-Yun	Enhancing The Performance of Amorphous IGZO Thin-Film Transistors Via Oxygen Plasma Treatment
P1.22	Zhang	Tiankai	Ion-modulated radical doping of triphenylamine-based semiconductors for efficient and stable hole transport layers
P1.23	Zhang	Qilun	Industrial Kraft Lignin Based Binary Cathode Interface Layer Enables Enhanced Stability in High Efficiency Organic Solar Cells.
P1.24	Solomeshch	Olga	SWIR Detectors based on Colloidal Quantum Dots
P1.25	ybakiewicz-Seki	Renata	Ambipolar derivatives of naphthalene diimides with oligo(ethylene glycol) chains for organic electrochemical transistors
P1.26	Shaposhnik	Polina	Application of C8-BTBT based EGOFETs at different acidity
P1.27	Stephens-Jones	Tristan	Computational Design of Bioinspired Materials for Organic Bioelectronics
P1.28	Kmentova	Iveta	Effect of the Structure of Bithienyl-Terminated Surfactants for Dielectric Layer Modification in Organic Transistor
P1.29	Yu	Hang	The Influence of Alkyl Spacers and Molecular Weight on the Charge Transport and Storage Properties of Oxy-Bithiophene-Based Conjugated Polymers

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POSTER SESSION 2 - October 3rd, 2023 18:00-19:30

P2.1	Eklund	Anni	Utilizing Electrochemical Surface Plasmon Resonance to control and observe ligand-receptor binding affinities
P2.2	Ghafari	Amir	Developing Stencil-Printed Organic Electrochemical Transistors for electrical characterization of responsive surfaces
P2.3	Smolka	Rastislav	Molecular Design of FR/NIR Emitting Materials for Bioimaging and Utilization of Host-Guest Mixtures as a Way of Increasing Fluorescence Intensity
P2.4	Zhang	Jie	The Design and Synthesis of Small Molecule Acceptor Materials based on N, S-heterocycles for Organic Solar Cells
P2.5	Huo	Chanyuan	Electrochemical Gating of Single-Molecule Junctions Utilizing the MCBJ Technique
P2.6	Tran	Van Chinh	Wood Electrochemical Transistor
P2.7	Omar	Omer H.	High-Throughput Virtual Screening of Existing Organic Chromophores for Materials Discovery
P2.8	Almulla	Latifah	Soft Photosensitive Polymers as Water-Compatible Soft Photosensitive Polymers as Water-Compatible Photodetectors
P2.9	Ricci	Gaetano	Exploring the electronic structure of extended triangulenes: opening new doors for a fast Reverse Intersystem Crossing
P2.10	Alsharif	Sarah	Organic/Inorganic Hybrid Detectors for Soft X-rays
P2.11	Prodhan	Suryoday	From monomer sequence to charge mobility in semiconductor polymers via model reduction
P2.12	Pataki	Nathan	A solution-processed micro-organic thermoelectric generator with record high thermocouple density
P2.13	Sadeghiyan	Maryam	Growth and multi-scale properties of hybrid magnetic tunnel junctions: towards the control of spinterfaces
P2.14	Tullii	Gabriele A. G.	Red light-induced modulation of cardiovascular cells physiology by conjugated polymers
P2.15	Masahiro	Ohara	A New Control Technique of Spontaneous Orientation Polarization: Observation of Orientation Relaxation by Rotary Kelvin Probe
P2.16	Singh	Anil Kumar	Spin-chirality interaction in transport through single molecule junctions
P2.17	Aloisio	Ludovico	Conductive thiophene-based fibers synthesized by living cells as novel bioelectronic materials
P2.18	Gajjar	Janvi V.	Structural, Electronic, and Electron transport property of Nickel-doped Porphyrin two-terminal device with graphene electrodes
P2.19	Mkhayar	Khaoula	In Silico Virtual Screening, Drug Likeness, ADMET, and Molecular Docking and Dynamics Studies for the Discovery of Potential Anti-Sleep Disorder Agents from In Silico Virtual
P2.20	Liu	Jinxu	Columnar Liquid Crystalline Corannulene with Axial Ferroelectricity
P2.21	Stein	Eyal	Ambipolar Blend-based Organic Mixed Ionic-Electronic Conductors
P2.22	Wollandt	Tobias	On the Extraction of Contact Resistance in Organic Thin-Film Transistors
P2.23	Scarano	Vincenzo	A new push-pull dye for semi-transparent p-type dye-sensitized solar cells
P2.24	Luukkonen	Axel	Performance and stability of IDT-BT water-gated thin-film transistors for use in biosensors
P2.25	asademont-Vina	Miquel	RAINBOW Organic Solar Cells: Implementing Spectral Splitting in Lateral Multi-Junction Architectures
P2.26	Tomita	Hiroki	Experimental study of the mechanism of the efficiency role-off due to triplet-polaron quenching in organic phosphorescent host-guest systems
P2.27	Beket	Gulzada	Vertical stratification and its impact on performance asymmetry of scalable laminated OPV devices
P2.28	Poimanova	Elena	Quantitative Determination of Influenza Virus by a Portable Device Based on EGOFET-Aptasensors
P2.29	Piscitelli	Matteo	Raman Spectroscopy of Electrolyte-gated graphene for protein detection

POSTER SESSION 3 - October 5th, 2023 18:00-19:30

P3.1	Yu	Hang	Towards a Deeper Understanding of the Ionic Charging in Naphthalenediimide-Based N-Type Conjugated Polymer Electrodes
P3.2	Mandal	Sougata	Electric Field Induced Negative Capacitance in Semiconducting Polymer
P3.3	Ke Liu	Xiao	Transport Layer Engineering Towards Lower Threshold for Perovskite Lasers
P3.4	Zhang	Huotian	Fill factor limit in organic solar cells
P3.5	Wenxin	Mao	Title in Arial, Bold, 16-Point Type and Centered, Upper and lower cases
P3.6	Dai	Yasi	Solvatochromic Emission from the “Dark” Double-Exciton State of a Polyhalogenated Thiele Hydrocarbon: a joint Quantum-Chemical and Experimental Investigation
P3.7	Funari	Riccardo	Influence of ligand exposure on the mechanical properties of biofunctionalized interfaces
P3.8	Palomino-Ruiz	Lucia	Substrate Transfer of Graphene Nanoribbons (GNRs): A Key Step in the Integration-to-devices Process
P3.9	Feng	Siyang	Donor-Acceptor-Donor Triads with Flexible Spacers: Deciphering Complex Photophysics for Targeted Materials Design
P3.10	Suranna	Gian Paolo	Simplified Fluorene-Based Hole Transport Materials for the Long-Term Stability of Perovskite Solar Cells
P3.11	Rashid	Umar	Mechano-reaction at a single molecular level: Forcing a Molecule to isomerize under application of external mechanical force.
P3.12	Butkute	Rita	Quinoxaline-based compounds for TADF emitters
P3.13	Lin	Yi	Molecular topology for the construction of organic semiconductor: design and synthesis
P3.14	Pavlica	Egon	High charge carrier mobility of multilayered random network of MXene flakes casted from water solution
P3.15	Hromadovà	Magdalèna	Quantum Interference Effect in Single Molecule Junctions Containing Multiple Aliphatic Bridges.
P3.16	Di Mario	Lorenzo	Outstanding Fill Factor in Inverted Organic Solar Cells with SnO2 by Atomic Layer Deposition
P3.17	Ali	Solgi	Enhancing Response Time in Organic Electrochemical Transistors via Top-Gate Configuration with Printed Solid-State Electrolyte
P3.18	Turco	Federico	Sustainable Carbon Dots with tunable optical properties as promising materials for agritech and green organic electronics
P3.19	Kasparavičius	Ernestas	Perovskite Solar Cells Investigation using A Kinetic Photoconductivity Method
P3.20	Squeo	enedetta Mar	Development of Water-Soluble Semiconducting Polar Polymers for Smart Applications
P3.21	Morris	James	Flicker noise analysis shows unusual oligoyne wire features
P3.22	Gentile	Giovanna	Semiconducting polymer bio-hybrid interfaces: characterization and first applications
P3.23	Wang	Yueyi	Accurate Mobility Extraction and Bias Stress Control via Novel Dual-Gate Four-Point-Probe Architecture
P3.24	Nijkoops	Annelot	π-Conjugated Food Derived Dyes for Artificial Retinas
P3.25	Garcia Romero	David	Understanding the Surface Chemistry of SnO2 Nanoparticles for High Performance and Stable Organic Solar Cells
P3.26	Alessandri	Riccardo	Machine Learning-Accelerated Multiscale Simulations of Redox-Active Polymers for All-Organic Energy Storage
P3.27	Khaliq	Aniqa	Extraction of force-distance curves in amplitude modulation atomic force microscopy
P3.28	Ziesel	Daniel	Inducing Overdrive Suppression in Chicken Cardiomyocytes Using Photovoltaic Devices and Multielectrode Arrays

P 1.1

Single-Component Squaraine Organic Upconversion Photodetectors with Peak Sensitivity at 1140 nm

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Laboratory for Functional Polymers, 8600 Dübendorf, Switzerland
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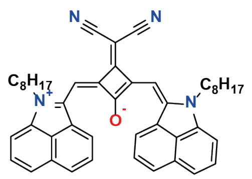
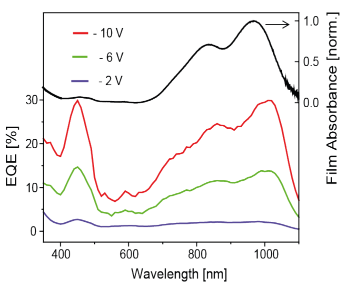
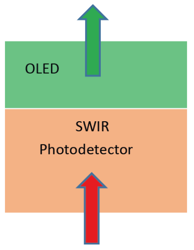
Optical sensing and imaging in the shortwave-infrared (SWIR) range of 900 – 1700 nm are essential to an increasing number of technologies in process control, machine vision systems, or medical imaging. For these applications, organic photodetectors (OPDs) attract attention because they can be processed cheaply from solution on flexible substrates, and can be integrated into wearable physiological monitors and next-generation SWIR sensing technologies. OPDs usually use a donor-acceptor combination of materials to split excitons into free charges due to their large binding energy. A disadvantage of this approach is that the use of a two-component blend film introduces morphological instability and a large processing space for device optimization. Therefore, from a design principle, fabrication, and optimization point of view, photoinduced charge generation in OPDs that consist of a single layer of active semiconducting material is highly appealing. In single-component OPDs, the challenge is to overcome the exciton binding energy. So far, very few single-component OPDs with sensitivity in the visible have been presented, but single-component SWIR-OPDs remained elusive.

We synthesized a series of new SWIR squaraine dyes with peak absorptions well beyond 1000 nm.[1] all dyes performed very well when integrated as a single layer in an OPD device architecture, with an external quantum efficiency for converting SWIR photons into electrical charges (EQE) over 30% at peak sensitivity wavelengths beyond 1100 nm. The EQE increased almost linearly with the strength of the (reverse) applied electric field, and the device response – both at the light switch-on and switch-off – was in the order of microseconds. We examined the charge-generation mechanism by varying the charge transport layers and performed a series of (transient) opto-electrical measurements, supported by numerical simulations. From these results, we conclude that photogeneration occurs intrinsically in the dye layer and that charges are not generated at an electrode-dye interface or are injected from the external circuitry via a trap-assisted photomultiplication mechanism. From simulations, we further conclude that charge generation is due to electric field-assisted dissociation of excitons, and the higher EQE under increased electrical field is not due to improved charge extraction.

We then fabricated so-called upconversion photodetectors (OUCs)[2] by combining the single-layer OPDs with a visible-emitting organic light-emitting diode (OLED). In an OUC, photogenerated charges generated inside the OPD by absorption of SWIR light are injected into the OLED, where they recombine under the emission of visible light. Thereby, an OUC converts a SWIR scene directly into a visible image.[3] The OUC performance metrics were impressive, with a turn-on voltage below 2.5 V and the maximum luminance on-off ratio was over 16000 at 4 V.


SWIR squaraine dye


Single-layer organic photodetector


Upconversion photodetector

References
[1] K. Strassel, et al., *Sci. Techn. Adv. Mater.* 2021, *22*, 194. [2] R. Hany, et al., *Sci. Techn. Adv. Mater.* 2019, *20*, 497. [3] W.-H. Hu, et al, *Adv. Opt. Mater.* 2022, *10*, 2200695.

P 1.2

Ytterbium Doping of Electron Transport Layer: Impact on Blue TADF-OLED Performance and Stability

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Balanced charge carrier transport and broad carrier recombination zone are essential for reducing triplet exciton concentration and suppressing triplet-mediated annihilation processes, which affect the performance and stability of blue-emitting organic light-emitting diodes (OLEDs) based on thermally activated delayed fluorescence (TADF).[1] Doping of organic layers is among the most effective methods to control these features. The doping of electron transport layer (ETL) with metals was demonstrated to be a promising option to facilitate electron injection, transport and improve charge balance.[2,3] While the case of lithium doping has been well-researched, ytterbium (Yb) doping has received less attention. The existing data is limited to electron injection characteristics, which are favored by the low work function of Yb (2.6 eV).[4]

Herein, the impact of Yb doping of ETL on the blue TADF-OLED performance, and particularly the lifetime, was thoroughly assessed. To this end, a series of OLEDs containing TmPyPB (as ETL) doped at different Yb ratios ranging from 0 to 30 wt% were fabricated and studied. It was found that the Yb-induced changes in the current density, which also affect device EQE, efficiency roll-off and luminance, result solely from alterations in electron current. The Yb-doping concentrations of 10 wt% or below was shown to reduce current density due to the electron trapping, whereas the higher doping levels indicated Yb-facilitated electron transport.

Most importantly, introduction of Yb extended blue-emitting device lifetime by 2 orders of magnitude compared to the undoped device, so that LT_{50} of the doped devices reached almost 800 and 50 hours at the luminance of 10^2 and $10^3 cd/m^2$, respectively. The enhanced device stability was attributed to Yb-assisted triplet exciton quenching, which occurred as a result of the recombination zone being in close proximity to the EML/ETL interface. The reduced triplet density in turn suppressed harmful triplet-mediated annihilation in EML and prolonged device lifetime, however, at the cost of somewhat deteriorated device efficiency.

References

[1] H. Nakanotani, K. Masui, J. Nishide, T. Shibata, C. Adachi, Sci. Rep. **3** (2013) 2127.

[2] J.H. Kwon, J.Y. Lee, Synth. Met. **159** (2009) 1292–1294.

[3] S.H. Choi, S.J. Lee, K.Y. Lee, H.S. Yang, K. Han, K.H. Kim, S.D. Kim, H.D. Bae, Y.H. Tak, Jpn. J. Appl. Phys. **48** (2009) 062101.

[4] H. Lee, H. Ahn, C. Lee, J. Kwak, J. Korean Phys. Soc. **61** (2012) 1536–1540.

P 1.3

Dithioketopyrrolopyrroles (DTPPs) as near-infrared absorbing n-type semiconductors

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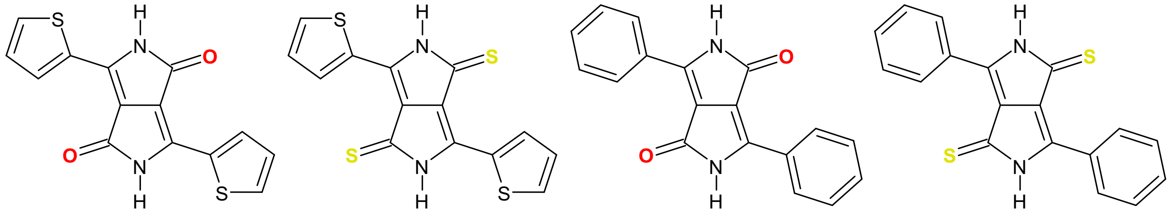
The diketopyrrolopyrrole derivatives (DPPs) belong to the major organic high-performance pigments finding several significant applications in diverse areas of organic electronics [1]. The core of these derivatives is formed by a molecule with the systematic name 2,5-dihydropyrrolo[4,3-*c*]pyrrolo-1,4-dione, which offers a wide range of possible structural modifications. One of the important derivatisations is the conversion of oxygen atoms in keto groups to sulfur atoms via one-step thionation using Lawesson's reagent [2]. In this work, basic thiophenyl (**Th-DPP**) and phenyl (**Ph-DPP**) DPP molecules were used as starting materials for the preparation of sulfur analogues **Th-DTPP** and **Ph-DTPP** (***Figure 1***), which were subsequently subjected to a study of electronic structure, optical and semiconducting properties.



Th-DPP **Th-DTPP** **Ph-DPP** **Ph-DTPP**

***Figure 1**: Chemical structures of the studied materials*

***Table 1**: Field effect mobilities of the studied materials*

Contact material		**Th-DPP**	**Th-DTPP**	**Ph-DPP**	**Ph-DTPP**
Al $[\mathrm{cm^2\cdot V^{-1}\cdot s^{-1}}]$	μ_e	$1.2\cdot10^{-5}$	**$7.4\cdot10^{-3}$**	$2.7\cdot10^{-3}$	**$1.8\cdot10^{-2}$**
Au $[\mathrm{cm^2\cdot V^{-1}\cdot s^{-1}}]$	μ_h	$2.0\cdot10^{-3}$	$4.9\cdot10^{-4}$	$6.6\cdot10^{-3}$	$3.0\cdot10^{-4}$

Thionation brought a bathochromic shift of the solid-state absorption edge. Furthermore, the electronic structure of the studied DTPPs showed low-lying, highly stabilised LUMO orbitals (–4.5 eV), which was in good agreement with model calculations, whereas the experimental HOMO destabilisation was significantly higher than predicted (–5.6 eV). Finally, field effect mobilities were determined on a bottom-gate top-contact transistor, where thionation caused the switching of the p-type character of DPPs to the n-type character of DTPPs (***Table 1***) [3]. Since DTPPs are still sufficiently thermally stable and have near-infrared absorption capability, low-lying LUMO and n-type mobility, they can be considered potential electron-accepting components in photovoltaics.

References

[1] M. Cigánek, J. Richtár, M. Weiter, J. Krajčovič, "Organic π-Conjugated Molecules: From Nature to Artificial Applications. Where are the Boundaries?", Isr. J. Chem. **61**, 1-15 (2021).

[2] F. Closs, R. Gompper, "2,5-Diazapentalenes", Angew. Chem. Int. Ed. Engl. **26**, 552-554 (1987).

[3] M. Kratochvíl, M. Cigánek, C. Yumusak et al., "Near-infrared absorbing hydrogen-bonded dithioketopyrrolopyrrole (DTPP) n-type semiconductors", Dyes Pigm. **197**, 109884 (2022).

P 1.4

Spectroscopy of Lumazine and Alloxazine in the Binary DMSO-Water Mixture

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The absorption and emission spectra were investigated for four molecules – lumazine and its cyanated derivative (Fig. 1. a) on the left) and alloxazine and its fluorinated derivative (Fig. 1. a) on the right), with dimethyl sulfoxide (DMSO) serving as the primary solvent. To modulate the spectroscopic properties, water was progressively added to the DMSO. Interesting effects were found, especially in the case of the cyanated derivative, where the addition of water results in a uniform blue shift, shown in Fig. 1. b). Further intriguing results were found for the samples containing 65 % of water and 35 % of DMSO. In this case, a notable decrease in absorption and emission intensities was registered, even larger than the water quenching observed in other cases. This is likely related to the formation of DMSO·$2H_2O$ trimers that has been documented in this case [1]. A similar behavior has been found for acetonitrile mixtures in the past, and a possible use for probing microenvironments of solvent immediately surrounding an analyte has been suggested [2].
Finally, water solubility is greatly enhanced by the substitution of polar groups, making it easier to penetrate cell membranes than the larger flavins, which have been used for fluorescence imaging of living cells [3]. Therefore, these molecules could find broader use for example in *in vitro* imaging.
The spectroscopic properties of studied molecules were calculated using the density functional theory in the implicit DMSO solvent model and with explicit water molecules.

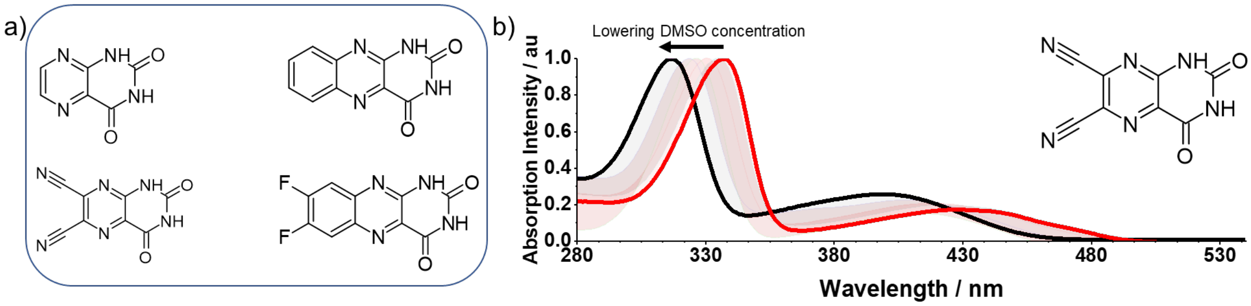

Fig. 1. a) the structures of the studied molecules; b) the effect of varying DMSO concentration on the absorption spectra.

References

[1] I. Płowaś, J. Świergiel, J. Jadżyn. Relative Static Permittivity of Dimethyl Sulfoxide + Water Mixtures. JCED **58**(6), 1741-1746 (2013).

[2] S. Dutta Choudhury, H. Pal. Intriguing Tautomerism of Lumichrome in Binary Aqueous Solvent Mixtures: Implications for Probing Microenvironments. JPC B **120**(46), 11970-11977 (2016)

[3] A. Golczak, M. Insińska-Rak, A. Davoudpour, et al. Photophysical properties of alloxazine derivatives with extended aromaticity – Potential redox-sensitive fluorescent probe. SAA 272, (2022).

P 1.5

Understanding the Effects of Processing Conditions on Non-Fullerene-Based Organic Photodiode Performances

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Organic photodetectors (OPDs) have gained significant attention due to their capability to absorb a broad spectrum of light frequencies, while being flexible, cost-effective, and suitable for various applications such as imaging, optical communications, sensing, and biomedical monitoring.[1] However, there are still significant challenges to overcome, including stability issues, morphology evolution, and difficulties in interface contact. Furthermore, even the most advanced OPD systems suffer from a substantial reduction in signal-to-noise ratio following light exposure.[2] Reducing dark current in OPDs is crucial for enhancing performance, and an important step towards achieving this is incorporating a suitable charge-selective interlayer during fabrication. However, this incorporation is not a simple process and requires a deep understanding of the physical processes occurring in the active layer and at the organic/metal interface, as well as determining the dominant mechanism for dark current generation.[3] Optimizing the implementation of the interlayer is crucial in order to accomplish dark current reduction and can be achieved through the addition of a suitable additive and morphology engineering.[4] Both of these steps are key in minimizing the unwanted minor charge carriers injection responsible for the noise currents, and achieving OPDs with excellent photo-sensing characteristics. We demonstrate that the introduction of a carefully chosen additive into a near-infrared (NIR) OPD system, along with morphology engineering, results in distinct behaviors concerning the collection abilities of charge carriers and the trends in dark current before and after illumination. This study highlights the significant impact of the additive's implementation method within the system on its influence on the electro-optical processes in the device. Additionally, it emphasizes the importance of employing appropriate processing conditions during fabrication, including thermal treatments, concentrations, and solvent selection, to achieve optimal results.

References

1.Fuentes-Hernandez, C. *et al.* Large-area low-noise flexible organic photodiodes for detecting faint visible light. *Science (1979)* **370**, 698–701 (2020).

2.Huang, J. *et al.* Understanding and Countering Illumination- Photodetectors with Reliable High Detectivity. (2021) doi:10.1021/acsnano.0c09426.

3.Simone, G., Dyson, M. J., Meskers, S. C. J., Janssen, R. A. J. & Gelinck, G. H. Organic Photodetectors and their Application in Large Area and Flexible Image Sensors: The Role of Dark Current. *Adv Funct Mater* **30**, (2020).

4.Vinokur, J. *et al.* Interlayers Self-Generated by Additive–Metal Interactions in Organic Electronic Devices. *Advanced Materials* **30**, 1–8 (2018).

P 1.6

Blending a Polyelectrolyte with a Mixed Ionic/Electronic Conducting Polymer for OECTs

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Bioelectronics is a rapidly growing field that relies on translating biological ion-based signals to readable electronic signals. Organic mixed ionic electronic conductors (OMIECs) are viable candidates for bioelectronics because they effectively support the transport and storage of ions and electrons, and are generally biocompatible. The most common strategy for OMIECs is that of a conjugated backbone that supports electron/hole transport, and sidechains that allow ion uptake and transport. Therefore, the arrangement of the polymer chains, i.e. the size, orientation and distribution of crystalline and amorphous domains, is expected to significantly affect OMIEC based devices. One way to control the OMIEC film morphology is by blending it with either small molecules or polymers.[1] We recently studied blends of poly(3-hexylthiophene-2,5-diyl) (P3HT), a common semiconducting polymer, and high molecular weight poly(ethylene oxide) (PEO), and found that optimal mixed conductivity is obtained at a “sweet-spot” composition. Morphology analysis showed that this composition contains sufficient PEO to support ionic conductivity and sufficient P3HT to provide high interfacial area between the polymers for ionic/electronic coupling.[2] Increasing the concentration of either component leads to phase separation that reduces the transport of either type of charge carrier. To enhance charge transport while attaining control of the morphology we investigated blends of P3HT, PEO and an OMIEC polymer, Poly(3-[2-(2-methoxyethoxy) ethoxy]ethylthiophene-2,5-diyl) (P3MEEET). We studied the effects of blend composition and the annealing temperature on the electrochemical behavior through spectroelectrochemistry (SEC) and electrochemical quartz crystal microbalance (EQCM) measurements, along with organic electrochemical transistor (OECT) device characterization for obtaining the transconductance and volumetric capacitance. Blend morphology and microstructure were determined using grazing incidence wide-angle X-ray scattering (GIWAXS) combined with High-Resolution Scanning Electron Microscopy (HRSEM). This correlation between composition, morphology and electrochemical performance provides insights into the design and integration of OMIEC polymers in bioelectronic applications.

References

[1]. Stein, E. *et al.* Ambipolar blend-based organic electrochemical transistors and inverters. *Nature Communications 2022 13:1* 13, 1–10 (2022).

[2]. Frankenstein, H. *et al.* Blends of polymer semiconductor and polymer electrolyte for mixed ionic and electronic conductivity. *J Mater Chem C Mater* 9, 7765–7777 (2021).

P 1.7

Preparation of nanographene by iterative organic synthesis

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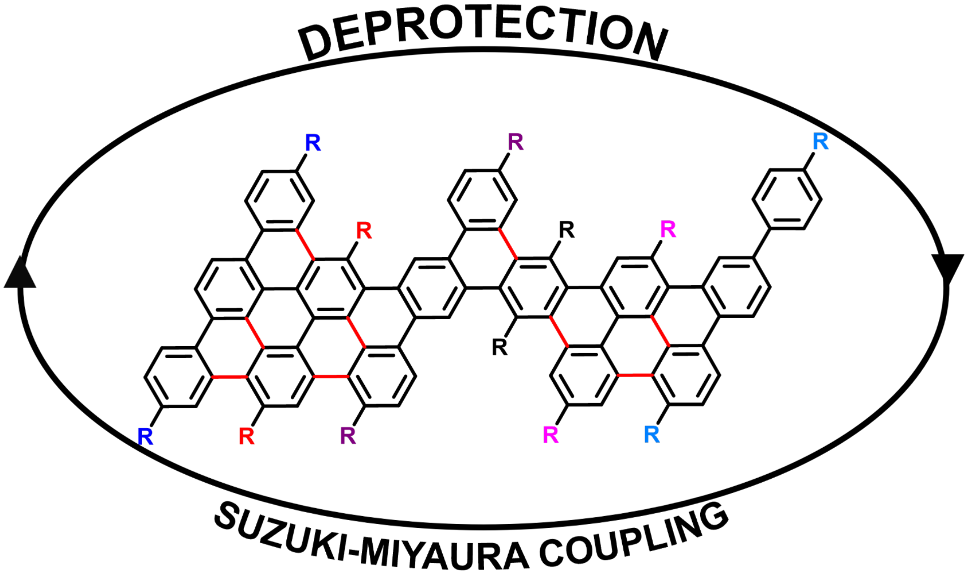
The structural precision of graphene nanoribbons is a key aspect as it significantly impacts their magnetic, optical, and electronic properties, particularly as the number of defects increases. Such alterations in properties can have profound implications for their prospective applications due to the considerable reduction in thermal and electrical conductance, critical properties for their use in electronic devices.[1]

In this project, the synthesis of graphene nanoribbons (GNRs) in solution will be conducted using an iterative Suzuki-type cross-coupling methodology. This iterative procedure will be accomplished by employing protective groups for the boronic acids functionalities, thus suppressing their capability to form new chemical bonds and enabling their selective removal as desired.[2] This iterative synthesis will permit the formation of monodispersed structures but simultaneously the introduction of different units creating a structurally heterogeneous nanoribbon.

In conclusion, our methodology will allow altering some of GNRs attributes such as their electronic properties and future applications in electronic devices. This system could be very useful for the automatization of the synthesis of nanographenes.



References

[1] A. Lennox, G. Lloyd-Jones, “Selection of boron reagents for Suzuki–Miyaura coupling,” Chem Soc. Rev. **43,** 412-443 (2014).
[2] Yin, J. et al. “Programmable Fabrication of Monodisperse Graphene Nanoribbons via Deterministic Iterative Synthesis,” J. Am. Chem. Soc. **144**, 16012–16019 (2022).

P 1.8

Graphitic Carbon Nitride Films for Electrical and Optical Applications

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The production of hydrogen as a clean energy source using abundant non-rare metal elements and visible light is an important strategy for the realization of a sustainable future. Graphitic carbon nitride (GCN) is a substance of great interest because it is composed only of carbon and nitrogen and shows a high photocatalytic activity for the splitting of water.[1] So far, GCN materials have been obtained as powders and utilized for these purposes. If GCN materials are available in the film form, what benefits one can obtain? The answer is clear considering that the science and technology of conductive polymers would not have emerged if polyacetylene was available only in the powdery form. In 2016, we have reported the first free-standing highly oriented GCN film by vapor deposition polymerization.[2] This GCN film is an insulator with the band gap of 2.7 eV. Here we report that the hybridization with a graphene-like structure can make the GCN film semiconducting with excellent electrical and optical properties. We will report details of these results.

References

[1] Xincheng Wang, Kazunari Domen, Markus Antonietti, *et al.*, "A metal-free polymeric photocatalyst for hydrogen production from water under visible light" *Nat. Mater*. **8**, 76–80, (2009).

[2] Hiroki Arazoe, Takuzo Aida, *et al.*, "An autonomous actuator driven by fluctuations in ambient humidity" *Nat. Mater.* **15**, 1084–1089, (2016).

P 1.9

Room-Temperature Operation of Vertical Tunnel Transistors with Organic Molecules as Quantum Dots

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Molecular-scale transistors hold promise for future nanoelectronics. An organic molecule has a regulated size on nanometer scale and thus exhibits attractive quantum transport which cannot be induced by inorganic quantum dots. In this regard, we have proposed a vertically-aligned molecular-scale transistor, where C_{60} molecules are utilized as quantum dots (Fig. (a)). [1] Of importance is that the molecules are fully isolated from each other and embedded in an insulating layer of a metal-oxide-semiconductor (MOS) structure. The MOS structure works as a double tunnel junction [2-4] and behave as a transistor channel. This feature of the transistor attains the quantum transport via a single or a few molecules in the vertical Si transistors, with the same analogy of scanning tunnelling spectroscopy.

We present a room-temperature operation of the vertical tunnel transistor. Although we demonstrated single-carrier transistor operations reflecting molecular orbitals in our previous work [5], the transistor operation was limited in a cryogenic temperature (20 K). In this study, we achieved the stable operation at 300 K by the optimization of the transistor structures including the distribution condition of the C_{60} molecules and the film thickness of the gate insulating layer. The drain current (I_D)–drain voltage (V_D) curves indicate clear staircases reflecting the molecular orbitals of C_{60} (Figs. (b) and (c)). The I_D values were markedly modulated by applying the gate voltages (V_G) even at 300 K. Furthermore, the transistor exhibited an ambipolar operation; namely n-type and p-type transistor operations were visible in the same transistor. The electron tunneling via the LUMO level enhanced by sweeping V_G from –8 to 8 V, indicating a n-type transistor operation (Fig. (b)). Whereas, the hole current through the HOMO level enhanced by applying the opposite V_G from 8 V to –8 V, which coincides with a p-type operation (Fig. (c)). These findings are benefits to achieve multivalued molecular circuits by a realistic way.

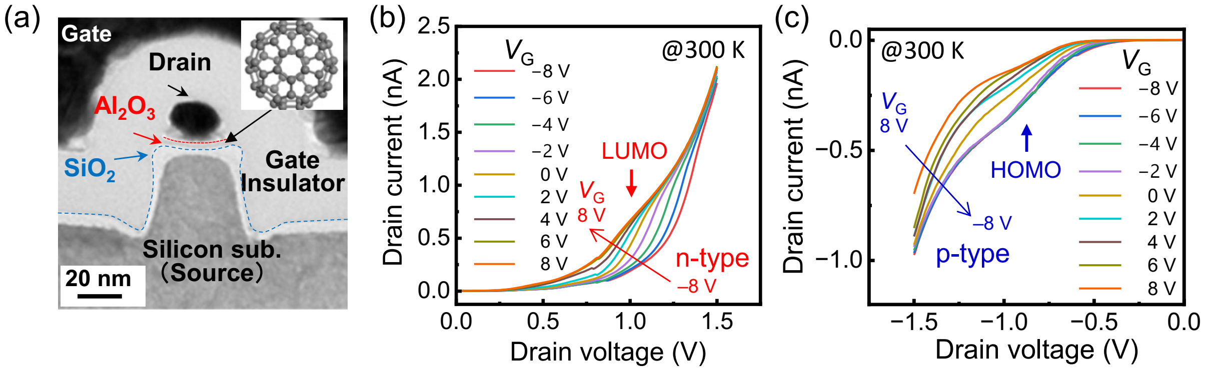

Figure (a) A transmission electron microscopy (TEM) image of a vertical tunnel transistor with C_{60} molecules as quantum dots. Reprinted from Ref. 1; copyright 2017, Royal Society of Chemistry. I_D–V_D curves of the vertical tunnel transistor obtained in (b) positive and (c) negative V_D range. The I_D–V_D curves were measured at 300 K.

References

[1] R. Hayakawa, T. Chikyow, Y. Wakayama, *Nanoscale* 9, 1129 (2017).
[2] R. Hayakawa, N. Hiroshiba, T. Chikyow, Y. Wakayama, *Adv. Funct. Mater.* 21, 2933 (2011).
[3] R. Hayakawa, K. Higashiguchi, K. Matsuda, T. Chikyow, Y. Wakayama, *ACS Appl. Matter. Interfaces* 5, 11371 (2013).
[4] H.-S. Seo, R. Hayakawa, T. Chikyow, Y. Wakayama, *J. Phys. Chem. C* 118, 6467 (2014).
[5] T. Basu, Y. Wakayama, R. Hayakawa, *ACS Appl. Electron. Matter.* 3, 973 (2021).

P 1.10

Quantum Chemical Calculations on Functionalized DTPs: Stable Components for Organic Semiconducting Materials

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Functionalized dithieno[3,2-b:2',3'-d]pyrroles (DTPs) represent highly interesting and frequently used multifunctional and electron-rich building blocks in organic semiconducting materials for application in organic electronic devices [1] or in polymeric form as electrode material in rechargeable batteries.[2]

We recently extended the scope of N-substituted DTPs resulting in a series of N-arylated and N-heteroarylated DTPs, which were subsequently implemented in functional materials for single material organic solar cells[3] or as hole transport material for perovskite solar cells,[4] respectively. By serendipity was found that by the proper choice of catalytic system and depending on the substitution at the DTP-nitrogen, novel differently substituted DTPs with N-aryl, unprecedented direct β-aryl, β,β‘-diaryl and α-aryl, α,α‘-diaryl scaffolds become available.[5] In this contribution, we address, with the help of quantum chemical calculations, the analysis of the geometry, electron density distribution and the correlation with the photophysical properties of the new family of compounds and explain the observed chemical selectivity of the reaction of unsubstituted and N-substituted DTPs with 9-anthracenyl halides.

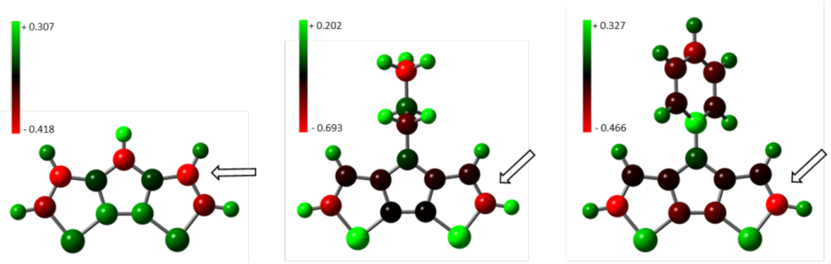

Figure 1: Calculated atomic charges distribution of some DTPs.

References

[1] X. Zhang, T. T. Steckler, R. R. Dasari, S. Ohira, W. J. Potscavage Jr., S. Prakash Tiwari, S. Coppée, S. Ellinger, S. Barlow, J.-L. Brédas, B. Kippelen, J. R. Reynolds and S. R. Marder, "Dithienopyrrole-based donor–acceptor copolymers: low band-gap materials for charge transport, photovoltaics and electrochromism", J. Mater. Chem. **20**, 123-134 (2010).
[2] P.-O. Schwartz, S. Förtsch, E. Mena-Osteritz, D. Weirather-Köstner, M. Wachtler and P. Bäuerle, "Ferrocene-functionalized polyheteroacenes for the use as cathode active material in rechargeable batteries", RSC Adv. **8**, 14193-14200 (2018).
[3] A. Vogt, F. Schwer, S. Förtsch, C. Lorenz, E. Mena-Osteritz, A. Aubele, T. Kraus and P. Bäuerle, "Broadly Applicable Synthesis of Arylated Dithieno[3,2-b:2′,3′-d]pyrroles as Building Blocks for Organic Electronic Materials", Chem. Eur. J. **27**, 12362-12370 (2021).
[4] C. Lorenz, A. Vogt, J. Millan, E. Mena-Osteritz and P. Bäuerle, "Broadly Applicable Synthesis of Heteroarylated Dithieno[3,2-b:2′,3′-d]pyrroles for Advanced Organic Materials – Part 1: Conducting Electropolymers", Org. Mater. **5**, 35-47 (**2023**).
[5] A. Vogt, F. Stümpges, J. Bajrami, D. Baumgarten, J. Millan, E. Mena-Osteritz and P. Bäuerle, submitted.

P 1.11

Hole transport in low-donor content organic solar cells: the role of the acceptor

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Thanks to the intensive research developed over the last years, the power conversion efficiency of organic solar cells (OSCs) surpassed 19%.[1] State-of-the-art OSCs make use of a donor-acceptor (D-A) structure, where holes and electrons are respectively transported after exciton splitting at the D-A interface. While this phenomenon is mostly taken for granted, special cases are challenging to describe. It was believed that to obtain an efficient charge extraction, both holes and electrons should find percolation paths formed by the donor and acceptor material, respectively. However, in 2011, Tang et al. reported a class of devices showing that this might not be exactly the case for every D-A structure.[2] The so-called low-donor OSCs delivered considerable performance, while using low donor concentration (TAPC, 5 wt%), for which a percolation path is not expected to be formed. The low-donor OSCs became an important model system for studying different properties due to the diminished morphological impact caused by the low donor concentration. However, the complete understanding of the operation mechanism in these systems is still under debate. Here, we investigate the hole transport mechanism in a set of low-donor bulk heterojunctions (BHJs). By varying the concentration of donor molecules dispersed into different acceptor matrices, we observed that the hole mobility is correlated with the $\mathrm{HOMO_D}$ – $\mathrm{LUMO_A}$ energy offset. This finding contradicts the expected behavior of these system predicted by the transport mechanisms suggested so far. Most of these mechanisms assume that the hole mobility is correlated with the $\mathrm{HOMO_D}$ – $\mathrm{HOMO_A}$ coupling and would, therefore, increase as these energy levels become close. From simulations we find that holes exploit the $\mathrm{LUMO_A}$ as virtual state in a superexchange process, which allows for hole transport even when percolation paths are not formed.

(1) Zhu, L. et al. Single-junction organic solar cells with over 19% efficiency enabled by a refined double-fibril network morphology. Nat Mater 21, 656–663 (2022)
(2) Zhang, M., Wang, H., Tian, H., Geng, Y. & Tang, Ching. W. Bulk Heterojunction Photovoltaic Cells with Low Donor Concentration. *Advanced Materials* **23**, 4960–4964 (2011)

P 1.12

Modification of work function of transparent conductive oxides by UV radiation

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Devices such as light-emitting diodes, solar cells (organic, hybrid, chalcogenide, tandem, etc.), field-effect transistors, etc. often consist of several layers. Each of the layers has its function: electrode, charge carrier blocking or transport layer, and the active layer. To create highly efficient devices, not only each layer is important, but their compatibility, too. Material energy level (ionization energy, work function (WF), electron affinity) compatibility will determine the efficiency of charge carrier flow in the device and thus the efficiency of the device itself. The most used methods for ionization energy level value measurements are ultraviolet (UV) photoelectron emission methods such as ultraviolet photoelectron spectroscopy (UPS) and photoelectron emission spectroscopy (PES).

It has been shown that the work function of transparent conductive oxides (TCO) can shift in UPS measurements. The effect has been related to the surface contamination and water layer reaction with the metal oxide due to the UV radiation [1,2]. However, in Kelvin Probe measurements, where surface contamination could be even more pronounced, no shift in work function was discovered.

The same shift we observed in PES when measuring the WF of indium tin oxide (ITO) and fluorine-doped tin oxide (FTO). By repeating the measurements, the WF shift of ~0.25 eV was obtained for ITO and FTO samples. As the PES method doesn't necessarily require a vacuum, the measurements were also done in the air. In that case, no WF shift was observed. Measurements in the air allow avoiding the WF shift during the measurements and the correct value can be obtained. Experiments and the obtained results will be discussed in more detail during the presentation.

References

[1] Schlaf, R. et al. J. Electron Spectros. Relat. Phenomena 120, 149–154 (2001)

[2] Beerbom, M. M. et al. J. Electron Spectros. Relat. Phenomena 152, 12–17 (2006)

P 1.13

Impact of thermally activated charge separation with offset non-fullerene acceptors

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Organic Solar cells have produced great excitement in the recent years with significant improvement in the power conversion efficiency (>19%) due to high charge generation yield and low voltage loss. However, the precise behaviour of charge generation and its corelation with energetic offset, in low voltage loss systems remain highly debated and questioned for numerous reasons. Here, we have studied the charge generation efficiency for wide range of donor:acceptor (D:A) system including low-offset and high-offset system. Surprisingly, we noted that charge generation is a temperature mediated process for low-offset systems and temperature-independent process for high-offset systems. The poor charge generation efficiency for low-offset system, which is further supported by transient absorption spectroscopy, is found to be increased by external thermal energy. Moreover, the charge generation activation energy (Ea) is also calculated and found that for an efficient charge generation at room temperature, the Ea should be less than the room temperature thermal energy, corelating well with the energetic offset between the donor and acceptor. The study also reveals that an increase in electrostatic dipole is the way forward to achieve the efficient charge generation without compromising on the voltage loss.

P 1.14

Energy level studies of self-assembling monolayer materials using photoelectron emission spectroscopy methods

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Two main factors will determine the efficiency of every solar cell: the charge carrier generation in the active layer and the charge carrier extraction from the cell itself. To improve the charge carrier extraction from solar cells, charge carrier transport layers are often used. Recently, self-assembling monolayers (SAMs) have become increasingly popular as charge carrier transport and/or extraction layers due to their low material consumption, relatively easy synthesis, and their ability to modify a work function of the electrodes to improve the energy level alignment at the interfaces. In this work, we have studied the energy level values of several SAM hole transport materials (HTMs). The chosen materials are based on a carbazole core with an attached phosphonic acid anchoring group.

The most popular method for ionization energy level determination is ultraviolet photoelectron spectroscopy (UPS). The equipment for this method is expensive as the measurements are done in ultra-high vacuum. A simpler and less costly method is a photoelectron emission spectroscopy (PES), where measurements can be performed either in the air or in a vacuum. Additionally, the scanning depth of more than 10 nm [1, 2] allows studying the SAM as well as the electrode simultaneously. In PES measurements it is possible to obtain a photoemission spectrum which is a sum of two spectra: electrons emitted from the electrode, and electrons emitted from the SAM. It is possible to separate the spectra and analyze each of them.

In this work we compare the ionization energy level values obtained from PES measurements of bulky films as well as the SAMs. Additional comparison was made with the previous energy level studies using UPS [3–5]. While there is no difference between SAMs and bulky films, there is a systematic difference between PES and UPS results.

The magnitude of ITO work function (WF) shift when it was covered with SAMs was compared to the surface potential changes obtained from scanning Kelvin probe measurements. In both cases, a correlation between the studied molecules' electrical dipole moment and the ITO WF shift was obtained.

In conclusion, the PES is a simple method to determine both the work function shift of the electrode and the ionization energy of the SAM material at the same time.

References

1. Grzibovskis, R. & Vembris, A. Study of the P3HT/PCBM interface using photoemission yield spectroscopy. in Organic Photonics VII vol. 9895 98950Q (2016).
2. Grzibovskis, R. & Vembris, A. Energy level determination in bulk heterojunction systems using photoemission yield spectroscopy: case of P3HT:PCBM. J. Mater. Sci. 53, 7506–7515 (2018).
3. Al-Ashouri, A. et al. Monolithic perovskite/silicon tandem solar cell with >29% efficiency by enhanced hole extraction. Science (80-.). 370, 1300–1309 (2020).
4. Al-Ashouri, A. et al. Conformal monolayer contacts with lossless interfaces for perovskite single junction and monolithic tandem solar cells. Energy Environ. Sci. 12, 3356–3369 (2019).
5. Lin, Y. et al. 18.9% Efficient Organic Solar Cells Based on n-Doped Bulk-Heterojunction and Halogen-Substituted Self-Assembled Monolayers as Hole Extracting Interlayers. Adv. Energy Mater. 12, (2022).

P 1.15

Understanding Contact Resistance In Nanoscale Organic Thin-Film Transistors

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Organic thin-film transistors (TFTs) show great potential for use in flexible electronics, including bendable and rollable active-matrix displays. Achieving better dynamic performance in organic TFTs requires minimizing the channel length, gate-to-contact overlaps and contact resistance to obtain a higher transit frequency [1]. However, the limit to which the critical lateral dimensions can be reduced depends on the patterning process. Most lithography methods, such as photolithography [2] and stencil lithography [3], have limited resolution of about 1 µm. We successfully fabricated flexible organic TFTs with dimensions as small as 100 nm using electron-beam lithography [4]. However, we found that the contact resistance of TFTs patterned by electron-beam lithography is more than an order of magnitude larger than that of TFTs fabricated using stencil lithography, despite using the same materials and device architecture. To understand the reason for this discrepancy, we performed atomic force microscopy and cross-sectional electron microscopy on organic TFTs patterned using both methods, and our findings indicate that the geometric angle of the edges of the source and drain contacts, which varies substantially based on the fabrication process, partially determines the contact resistance. Stencil lithography produces extremely shallow edge angles (~1°), leading to low contact resistance (~0.1 kΩcm), while electron-beam lithography produces sharp edge angles (~40°), causing higher contact resistance (>1 kΩcm). We found that by modifying the contact-metal deposition process, it is possible to decrease the edge angle in TFTs patterned by electron-beam lithography from 40° to about 10° and thus the contact resistance to about 0.5 kΩcm.

References

[1] U. Zschieschang et al., "Roadmap to Gigahertz Organic Transistors," Advanced Functional Materials **30**, 1903812 (2020).

[2] T. Sawada et al., "Correlation between the static and dynamic responses of organic single-crystal field-effect transistors," Nature Communications **11**, 4839 (2020).

[3] A. Perinot et al., "Accessing MHz operation at 2 V with field-effect transistors based on printed polymers on plastic," Advanced Science **6**, 1801566 (2019).

[4] U. Zschieschang et al., "Nanoscale flexible organic thin-film transistors," Science Advances **8**, eabm9845 (2022).

P 1.16

Highly-oxidised indolocarbazoles: ideal open-shell candidates for single-molecule electronics

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Several studies have highlighted the promise of open-shell (radical) materials in single-molecule electronics, especially to increase charge transport efficiency[1] or to boost thermoelectric energy harvesting. In our ongoing search for open-shell species that can be assembled as single-molecule junctions, we focussed our efforts on the indolocarbazole family. This includes a variety of natural and synthetic compounds which have been widely studied for their outstanding physico-chemical properties, which include narrow HOMO-LUMO gap and existence of multiple redox state[2]. The latter include the possibility of oxidation to a radical cationic state and even to a highly reactive diradical dication, making them ideal candidates for single-molecule transport studies.

We synthesised a N,N-disubstituted indolocarbazole (Fig. 1a), with aurophilic thioanisolyl substituents on the two pyrrolic N, and fully characterised its photochemical and electrochemical behavior (Fig. 1b). We then measured its single-molecule conductance with the Scanning Tunnelling Microscope – Break Junction (STM-BJ) technique, which returned a value of $10^{-5.15}$ G_0 (Fig. 1c and d). Our initial characterisation shows the promise of this system, and we are working now on the isolation of the oxidised form (radical cation and diradical dication) by chemical means, which will be followed by the determination of their single-molecule charge transport. These data will be compared with those obtained by in-situ oxidation by Electrochemically-Controlled STM-BJ in a four-electrode apparatus. The two approaches combined will yield valuable information on the mechanism of charge transport and the suitability of indolocarbazole compounds to further studies in molecular thermoelectrics.

We shall report on this data and the current, undergoing experiments at the meeting.

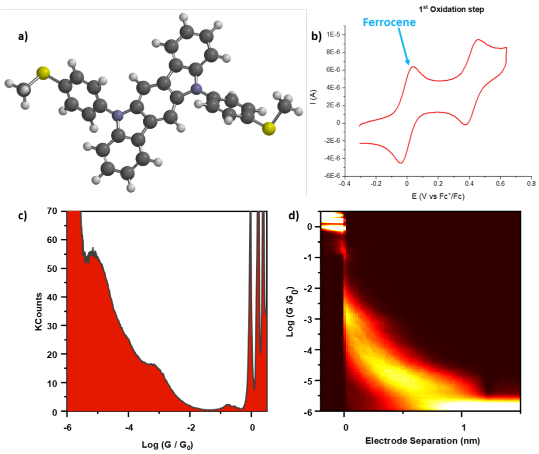

Figure 1

References

[1] Jonathan S. Ward, Andrea Vezzoli "Key advances in electrochemically-addressable single-molecule electronics", Curr. Opin. Electrochem. **35,** 101083-101089 (2022).

[2] Tomasz Janosik, Agneta Rannug, Ulf Rannug, Niklas Wahlström, Johnny Slätt, Jan Bergman "Chemistry and Properties of Indolocarbazoles", Chem. Rev. **118**, 9058-9128 (2018).

P 1.17

Thermally activated delayed fluorescent organic scintillators for high resolution X-ray imaging

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Abstract

The research on developing organic scintillators flourished, aiming at integration with high-performance photodetectors for high resolution imaging applications. Given the great progresses, efforts on searching for highly sensitive, fast-responsive, small-sizable, and cost-effective X-ray detectors are on-going, which can produce devices exhibiting extremely low-dose and high-resolution X-ray detection capability. However, comparing to their inorganic counterparts, traditional organic materials are not ideal X-ray scintillators considering they contain light elements which absorbed less X-ray and convert less X-ray into visible light. Additionally, owing to the generation of multiple triplet exciton under X-ray scintillation, the loss of utilization of triplets leads to low light yield value. To address these issues, pioneer works on purely organic room temperature phosphors,[1] TADF emitters for X-ray scintillation had been reported.[2] Further challenge lies in simultaneously realizing both moderate X-ray absorbance while maintaining decent optical properties. In our project we addressed the above issues by introducing heavy atoms into the molecular backbone without sacrificing their PLQYs. Utilizing D-A largely twisted molecular design paradigm, efficient utilization of ‘dark’ triplets was realized via a fast reverse intersystem crossing channel. Adopting such a strategy, significantly enhanced RL intensity (almost 10 times) can be achieved in contrast to those of the traditional organic scintillators.

References

[1] J.-X. Wang, etc., “Heavy-atom engineering of thermally activated delayed fluorophores for high-performance X-ray imaging scintillators,” Nature Photonics 2021, **15**, 187-192.

[2] W. Ma, etc., “Thermally activated delayed fluorescence (TADF) organic molecules for efficient X-ray scintillation and imaging” Nature Materials 2022, 21, 210-216.

P 1.18

Impact of long-term voltage cycling on functionalized thiol-SAM electrodes in EGOFET-based applications

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Electrolyte-gated organic field-effect transistors (EGOFETs) have been used as high-performance biosensors [1] with long-term usability for multiple measurements on one device [2]. This suggests a need to quickly establish reference point for certain electrical parameters, such as threshold voltage, to which the biosensing measurements can be compared. It is also important to ensure that the device itself is stable before, during and after sensing to avoid false results. A reference gate electrode which monitors the transistor itself outside of sensing measurements is therefore often used. A bare gold surface as a reference electrode might introduce surface reactions and oxidations [2], leading to undesired faradaic currents. A way to minimize these issues is to passivate the gold surface in contact with the electrolyte by using a self-assembled monolayer.

In this work, we have studied thermally deposited gold electrodes functionalized with SAMs based on three different n-alkanethiols: propanethiol (C3), hexanethiol (C6) and octanethiol (C8). We investigated the impact long-term, repeated voltage cycling has on these three different SAMs through a series of different measurements and characterization techniques, including FET transfer characteristics, cyclic voltammetry (CV), and X-ray photoelectron spectroscopy (XPS).

Transfer characteristics and the impact of long-term voltage cycling were studied with two different measurement setups: with the functionalized thiol-SAM electrodes as i) a gate in an EGOFET and ii) as an extended gate to a MOSFET. Electrical parameters extracted and studied from these measurements include threshold voltage and hysteresis, both of which are dependent on the gate electrode surface. To ensure the stability of the thiol-SAMs and to rule out any desorption of thiol molecules during these measurements, XPS analysis was performed before and after select measurements. The results are consistent with previously suggested models for electrical transport across such SAMs [3], confirming that these monolayers restrict faradic processes at the electrodes by passivating the Au surface.

References

[1] Macchia, Eleonora, et al. "Single-molecule detection with a millimetre-sized transistor." *Nature communications* 9.1 (2018): 3223.

[2] Luukkonen, Axel, et al. “Long-term electrical characteristics of a poly-3-hexylthiophene water-gated thin-film transistor”. *Organic Electronics*, accepted for publication (2023).

[3] Gupta, Chaitanya, et al. "Electronic Properties of a Monolayer− Electrolyte Interface Obtained from Mechanistic Impedance Analysis." *The Journal of Physical Chemistry C* 113.21 (2009): 9375-9391.

P 1.19

Experimental and theoretical study of exciplex-forming compounds containing trifluorobiphenyl and 3,6-di-tert-butylcarbazole units and their performance in OLEDs

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Nowadays, computational guiding of molecular design is vitally required for the fast and efficient development of advanced materials. Many articles were reported on the computational studies of donor-acceptor molecules with small differences of energies of excited singlet and triplet states required for the realization of thermally activated delayed fluorescence (TADF) [1]. Despite TADF can be observed from the solid mixtures of simple exciplex-forming electron-donating and electron accepting molecules, computational guiding for their molecular design has not attracted much attention yet. In this combined theoretical and experimental study, a computational protocol using default and tuned ω parameter will be reported to predict the excited states, molecular geometries, and electronic structures of efficient blue exciplex-forming compounds with donor-acceptor structure containing trifluorobiphenyl acceptor moiety and 3,6-di-tert-butylcarbazolyl donor groups. They show high but different triplet and singlet energies and high singlet-triplet splitting. To prove the theoretical concepts, very simple but perfect for efficient blue exciplex-based TADF derivatives of trifluorobiphenyl and 3,6-di-tert-butylcarbazole were synthesised and characterized as exciplex-forming donors for electroluminescent devices.

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References

[1] A. K. Narsaria, F. Rauch, J. Krebs, P. Endres, A. Friedrich, I. Krummenacher, T. B. Marder, „*Computationally Guided Molecular Design to Minimize the LE/CT Gap in D-π-A Fluorinated Triarylboranes for Efficient TADF via D and π-Bridge Tuning*", *Adv. Funct. Mater*. **31**, 2002064 (2020).

P 1.20

Blue-emitting Carbon Quantum Dots from Hydrothermal Approach: Purification Strategies Comparison and Influence of the Reaction Parameters on the Spectroscopic and Electrochemical Properties.

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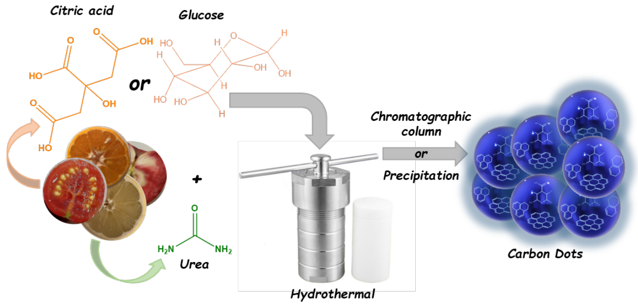
In recent years research studies on carbon quantum dots (CDs) were characterized by rapid development, because of their peculiar optical properties, facile preparation, and modification, absence of heavy metals, and excellent biocompatibility, which make them suitable materials for a plethora of applications going from sensing to nanomaterials phototheranostics, bioimaging, and optoelectronic devices[1]. However, besides the numerous studies on the argument, the reaction products of the CDs synthesis process, mainly consist of mixtures composed of different CDs fractions, reaction intermediates, and side products, which may hamper the analysis of both the structural and optical properties of the materials[1,2]. Thus, the separation and purification strategies of CDs may play a crucial role in the reliable characterization of these materials. Among the different purification methods, the precipitation one is suitable for large-scale preparation of CDs, while chromatographic techniques could be an alternative approach to separate CDs into fractions of different particles size. Starting from those considerations, here we selected the hydrothermal approach to preparing blue-emitting CDs, owing to its feasibility for large-scale industrial applications. We employed precursors which could be obtained from biowaste, like citric acid (CA) or glucose (Glu) as carbon sources and urea as both base and nitrogen sources (Scheme 1). Through absorption spectroscopy and photoluminescence emission analyses, we compared the precipitation method and the chromatographic column one, and we observed no marked differences. Then we studied the influence of the precursors and the reaction temperature on the spectroscopic and electrochemical properties of the post-treated CDs.



Scheme 1. Reaction scheme for CDs synthesis.

References

[1] H. Lin et al., "*Study and Comparison on Purification Methods of Multicolor Emission Carbon Dots*", Chem. As. J. **16**, 348-354 (2021).

[2] B. Vercelli, B. La Ferla, *"Red-Emitting Carbon Quantum Dots for Biomedical Applications: Synthesis and Purification Issues of the Hydrothermal Approach",* Nanomaterials **13(10)**, 1635 (2023).

P 1.21

Enhancing The Performance of Amorphous IGZO Thin-Film Transistors Via Oxygen Plasma Treatment

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Amorphous indium-gallium-zinc-oxide (a-IGZO) films are attractive active layers for high performance electronic switching elements such as thin-film transistors (TFT) due to their atmospheric and operational stability. Moreover, a-IGZO has very high transmittance in the visible range, which makes it an ideal candidate to be used in displays or next generation IoT and embedded devices such as mirrors, clothes or augmented reality devices.

In this work we present significant improvement in the electrical characteristics of a 50 nm-thick a-IGZO layer deposited by radio-frequency (RF) sputtering after employing oxygen plasma treatment. After formation, the active layer was thermally annealed at 300 °C for 1 hour before beginning the oxygen plasma treatment. The effects of the plasma generator RF power were studied at 60, 120 and 180 W. The oxygen plasma was found to affect the optical absorption, surface roughness and the atomic composition of the thin film as well as the device performance of the TFTs based on the a-IGZO layers. The on/off current ratio and subthreshold swing improved significantly after the treatment compared to the device with the as-deposited a-IGZO layer. For the charge carrier mobility and threshold voltage however, the devices treated with oxygen plasma generated at 60 W showed the best performance, and both parameters have deteriorated at higher RF powers. Interestingly, at 180 W the mobility was reduced to and the threshold voltage increased over than that of the device with the as-deposited a-IGZO. The X-ray photoelectron spectra of the thin films were analyzed. It was found that the a-IGZO treated with oxygen plasma at 60 W RF power has the lowest ratio of OH groups which are often related to charge trapping in metal-oxide semiconductors. The optical band gap, as extracted from the Tauc plot, is the highest of this thin film, further suggesting decreased trap density, confirming the effect of traps on device performance. The atomic force microscope imaging showed that the surface roughness significantly decreases after the plasma treatment. This might explain the sharp improvement in the subthreshold swing, which is influenced by surface-related charge trapping.

This study shows that the post-deposition oxygen plasma treatment of RF sputtering-deposited a-IGZO active layer is an effective way to enhance TFT performance by inducing favorable changes in the physical properties of the metal-oxide film.

References

[1] W. Wu, L. Zhang, Z. Xu, L. Zhou, H. Tao, J. Zou, M. Xu, L. Wang, J. Peng, IEEE Trans. Electron Devices **64**, 1991 (2017).
[2] J. C. Park, S. Kim, S. Kim, C. Kim, I. Song, Y. Park, U.-I. Jung, D. H. Kim, J.-S. Lee, Adv. Mater. **22**, 5512 (2010).
[3] S. Jeon, S.-E. Ahn, I. Song, C. J. Kim, U. I. Chung, E. Lee, I. Yoo, A. Nathan, S. Lee, K. Ghaffarzadeh, J. Robertson, K. Kim, Nat. Mater. **11**, 301 (2012).
[4] E. Song, B. Kang, I. Han, K. Oh, B. Kim, H. Nam, IEEE Elect. Device Lett. **36**, 247 (2015).

P 1.22

Ion-modulated radical doping of triphenylamine-based semiconductors for efficient and stable hole transport layers

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Organic semiconductors (OSCs) have been widely applied as the charge transport layers in perovskite solar cells (PSCs) owing to their low-temperature and solution processability. In charge transport layer applications, efficient doping of the OSCs plays the most key role in optimizing device performance through significantly modifying the conductivity and energetic levels. However, state-of-the-art OSCs (e.g. spiro-OMeTAD[1], PTAA[2]) used as hole transport layers in PSCs suffer from limited doping efficiency and poor stability. In this work, by investigating the doping process of radical doped[3] triphenylamine-based p-type OSCs, we revealed that the doping efficiency saturation is due to the Coulomb interaction between the hole polaron and counter ion in radical dopant. By further incorporating organic ionic salts into the radical doped OSCs system, the strong Coulomb interactions between hole polaron and counter ion can be effectively screened, which promote the delocalization of the hole polaron and thus the increase of the doping efficiency. By molecular designing of the organic ionic salts, the doping stability can also be improved. With this new ion-modulated radical doping strategy, we achieved PCEs of >25% and much-improved device stability under harsh conditions[4]. In addition, this ion-modulated radical doping strategy can effectively decouple conductivity and WF tunability, inspiring further optimization in other optoelectronic devices.

References

[1] U. Bach et. al., *Solid-state dye-sensitized mesoporous TiO_2 solar cells with high photon-to-electron conversion efficiencies*, Nature, **395**(6702): 583-585 (1998).

[2] Y. Wang, et al. *PTAA as efficient hole transport materials in perovskite solar cells: A review*, Solar RRL, **6**(8): 2200234 (2022).

[3] W. H. Nguyen et. al., *Enhancing the hole-conductivity of spiro-OMeTAD without oxygen or lithium salts by using spiro(TFSI)$_2$ in perovskite and dye-sensitized solar cells*, J. Am. Chem. Soc. **136(**31), 10996-11001 (2014).

[4] T. Zhang et. al., *Ion-modulated radical doping of spiro-OMeTAD for more efficient and stable perovskite solar cells*, Science, **377**(6605), 495-501 (2022).

P 1.23

Industrial Kraft Lignin Based Binary Cathode Interface Layer Enables Enhanced Stability in High Efficiency Organic Solar Cells.

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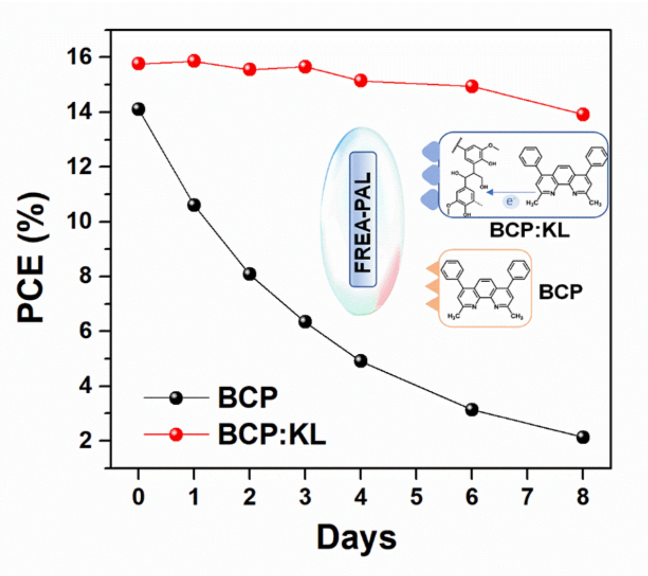
Herein, a binary cathode interface layer (CIL) strategy based on the industrial solvent fractionated LignoBoost Kraft lignin (KL) is adopted for fabrication of organic solar cells (OSCs). The uniform-distributed multiple phenol enables KL to easily form bonds with commonly used CIL materials, i.e., bathocuproine (BCP) and PFN-Br, resulting in binary CILs with tunable work function (WF). The binary CILs work well in OSCs with large KL ratio compatibility, exhibiting equivalent or even higher efficiency to the traditional CILs in state of art OSCs. In addition, the combination of KL and BCP significantly enhanced OSC stability, owing to KL blocking the reaction between BCP and non-fullerene acceptors (NFAs). This work provides a simple and effective way to achieve high-efficient OSCs with better stability and sustainability by using wood-based materials.



References

[1] Jawerth, Marcus E., et al. "Mechanical and morphological properties of lignin-based thermosets." ACS Appl. Polym. Mater. **2.2** 668-676 (2020).

[2] Liu, Tiefeng, et al. "Bathocuproine as a cathode interlayer for nonfullerene organic solar cells with efficiency over 17%." J. Mater. Chem. A **9.40** 23269-23275 (2021).

[3] Song, Hang, et al. "Hybrid cathode interlayer enables 17.4% efficiency binary organic solar cells." Adv. Sci. **9.8** 2105575 (2022).

SWIR Detectors based on Colloidal Quantum Dots

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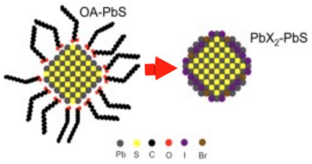
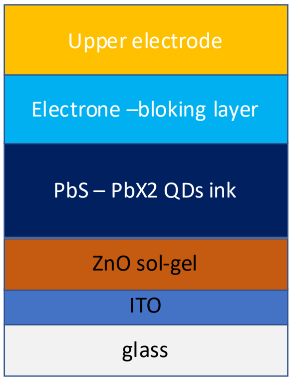
Results of the study sensitive organic-inorganic devices with the structure: Glass/ITO/ZnO/PbX_2-PbS/EBL/upper electrode have been presented. 4 - pixels substrates (1.4 sm x 1.4 sm) were fabricated from Glass - ITO samples by photo-lithography method in Technion's micro-nano fabrication & printing unit (MNF&PU). PbS core-type quantum dots (QDs), with original concentration C=10 mg/mL in toluene and a fluorescence peak at λ_{em} 1200 nm were, first, surface passivated in air by ligands PbX_2, where $X_2 = I_2$ and Br_2, by exchange method, as shown on the Scheme. The resulting (PbS-PbX_2) ink was spin-coated on 4-pixels ITO substrate, followed by a fabrication of ZnO sol-gel layer. The different types of upper electrodes have been thermal deposited through a shadow mask on the working layer. For optimization of device performance, fluorinated fullerene $C_{60}F_{48}$ was also applied to organic electron-bloking layer (EBL) as p-dopant. The structure of devices has been presented on Figure. Dark – light photovoltaic characteristics of devices, the effect of organic EBL and bias dependent on the external quantum efficiency (EQE) have been studied.

The Scheme of the surface passivation of PbS QDs in air by ligands exchange to PbX_2, where $X_2 = I_2$ and Br_2



The structure of Organic-inorganic devices, based on PbS quantum dots:

Glass/ITO/ZnO/PbS/EBL/upper electrode



P 1.25

Ambipolar derivatives of naphthalene diimides with oligo(ethylene glycol) chains for organic electrochemical transistors

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Organic electrochemical transistors (OECTs) represent a promising category of semiconductor devices, owing to their dual conduction nature: electronic and ionic. This unique characteristic enables their utilization in rapidly evolving fields such as neuroprosthetics, implantology, and biomedicine in recent years. The current challenge in scientific research is to propose novel OECTs that not only possess competitive electrical parameters but also exhibit high stability in a water working environment. Within the scope of this study, three amphiphilic donor-acceptor compounds were designed and synthesized. To achieve this, the central naphthalendiimide (NDI) unit was symmetrically substituted with electron donor groups, namely carbazole (Carb), dithienopyrrole (DTP), and diethylenedioxathiophene (BEDOT) (Figure 1). The conducted spectroscopic and electrochemical analyses facilitated the determination of the influence of the applied electron donor unit on the optical and electronic properties of the resulting materials. All synthesized compounds underwent electropolymerization, leading to the formation of polymers that exhibited electroactivity in both organic and aqueous electrolytes. Through spectroelectrochemical measurements and electrochemical impedance spectroscopy (EIS) studies, the most promising electrode material, poly(G-DTP-G-NDI), was selected. This material was subsequently employed as the active layer in the construction of OECTs with a vertical architecture. The obtained results verified the ambipolarity of the transistor and its stability during aging tests.

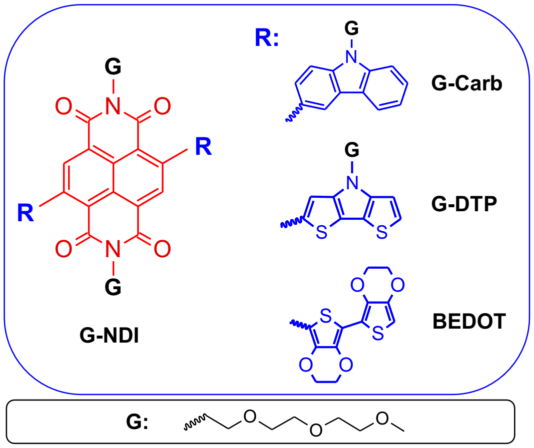

Figure 1. Structural formulas of the synthesized naphthalene diimides derivatives.

Acknowledgement
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P 1.26

Application of C8-BTBT based EGOFETs at different acidity

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Electrolyte-gated organic field-effect transistors (EGOFETs) are organic electronic devices, which are intensively developed for sensing in aqueous media and neuromorphic applications. EGOFETs as a platform for biosensing devices enable detecting biological molecules in down-to-attomolar range [1]. However, the operation of biosensors is hindered with some difficulties, one of which is non-specific interactions between particles of the analyzed solution and device interfaces. In our work, we have focused on proton interactions with organic semiconducting (OSC) layer of EGOFETs because protons are a sort of particles that always present in biological solutions [2]. The proton concentration could significantly vary in such physiological solutions as urine and sweat. For this purpose 2,7-dioctyl[1]benzothieno [3,2-b]benzothiophene (C8-BTBT) was chosen as the OSC material because it is well-known for high stability and charge carriers mobility. A blend of C8-BTBT and polystyrene was used to suppress 3D molecules aggregation and obtain flat crystals of the OSC (Fig. 1,a) [3].

Electrical characteristics of the device was investigated by acid addition to a neutral electrolyte solution. The threshold voltage was not changed until pH = 4.9, however, it showed a positive shift with the average pH sensitivity of 62 mV/pH in the range from pH 4.9 to pH 2.8 (Fig 1,b). Whereas the off current demonstrated the very similar type of pH dependence, the transconductance weakly decreased during the acid addition, which means that the charge carrier mobility was not improved. Such dependency was observed for two different types of the substrates (Si/SiO_2 and PEN) and different counter ions (Cl^- and p-toluenesulfonic cation). It allowed suggesting the following mechanism of proton interactions with C8-BTBT molecules: a proton attach to a free electron pair of the sulfur atom of BTBT and act as a localized deep trap healer, whereas shallow trap healing does not take place (Fig 1,b).

In order to check the applicability of the EGOFETs in a flow mode, a flow chamber was designed and assembled. The preliminary results obtained in the flow mode measurements showed a fast response to pH variations.

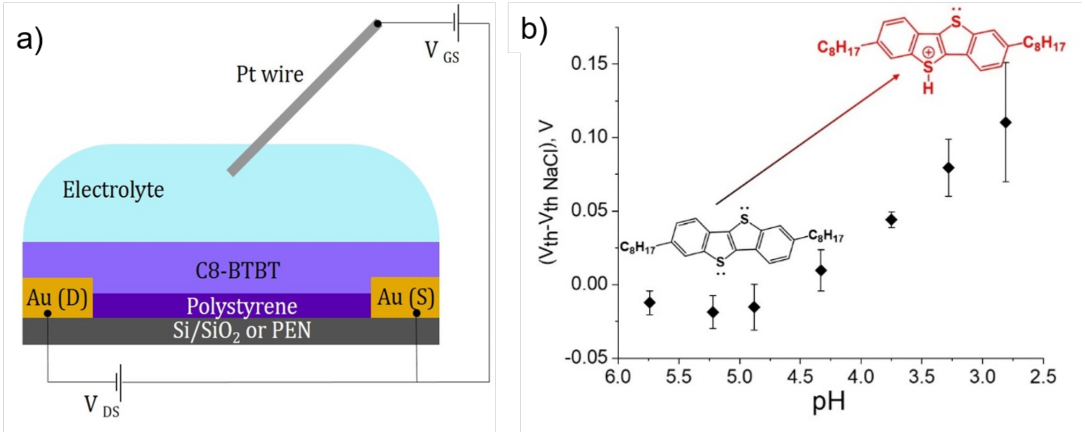

Figure 1. (a) The EGOFET device layout; (b) pH dependence of the device.

This work was supported by the Russian Science Foundation (grant 19-73-30028-P).

1. E. Macchia et al., *Flex. Print. Electron.*, **2018**, *vol. 3*, 034002.
2. P. Shaposhnik. et al., *Chemosensors*, **2023**, *vol.11*, 74.
3. P. Shaposhnik. et al., *Dokl. Phys. Chem.*, **2021**, vo*l. 496*, pp. 20–24.

P 1.27

Computational Design of Bioinspired Materials for Organic Bioelectronics

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Bioinspired organic polymers have shown great potential in recent years in the area of bioelectronics. Devices so far have used existing organic semiconductors and then functionalised to make them more hydrophilic, but they have shown poor biocompatibility and poor long-term operational stability.[1]

Therefore, this research employs computational/in silico screening tools of bioinspired building blocks. It investigates their potential use as the next-generation materials for bioelectronics by leveraging sustainable design and predictors for aggregation/order, ionic and electronic transport properties. This will be achieved by exploring the combination of different bioinspired moieties to create motifs of different conjugated units. The motifs that show promising electronic/protonic transport will undergo further study by exploring different linkers and side chains to alter their chemistry.

Melanin-inspired units were used as a '*proof of concept*'. This is because melanin is a bioderived conducting material which has been shown to have promising electronic and protonic transport.[1, 2] Therefore, Indole-substituted (melanin-inspired) fragments and common heterocyclic conjugated building blocks (that are found in organic electronics) were selected from literature and patent databases.[3-6] The electron-rich, melanin building blocks were then combinatorially assembled with the conjugated fragments to produce dyads. This strategy was employed to increase the electronic transport and ordering in the melanin.

Density Functional Theory (DFT) calculations were then used to produce a set of descriptors that screen the electronic and conformational properties. The acceptor/donor pairs that show promising electronic properties undergo further study. This involves producing longer oligomers from the dyads. As well as altering the linkers between the fragments so to improve the desirable properties such as a customizable band gap. Finally, the oligomers also undergo sidechain optimization so to improve their solubility, processability and morphology.

References

1. A.B. Mostert, *Polymers*, 2021, **13**, 1670
2. F. Solano, *IJMS*, 2017, **18**, 1561
3. B. D. Paulsen, et al., *Nat. Mater.*, 2020, **19**, 13–26.
4. Z. Huang, et al., *Chem. Int. Ed.*, 2018, **57**, 11963–11967.
5. W. R. Pitt, et al., *J. Med. Chem.*, 2009, **52**, 2952–2963.
6. L.-P. Boivin, et al., *Macromolecular Chemistry and Physics*, 2022, **224**, 2200378.

P 1.28

Effect of the Structure of Bithienyl-Terminated Surfactants for Dielectric Layer Modification in Organic Transistor

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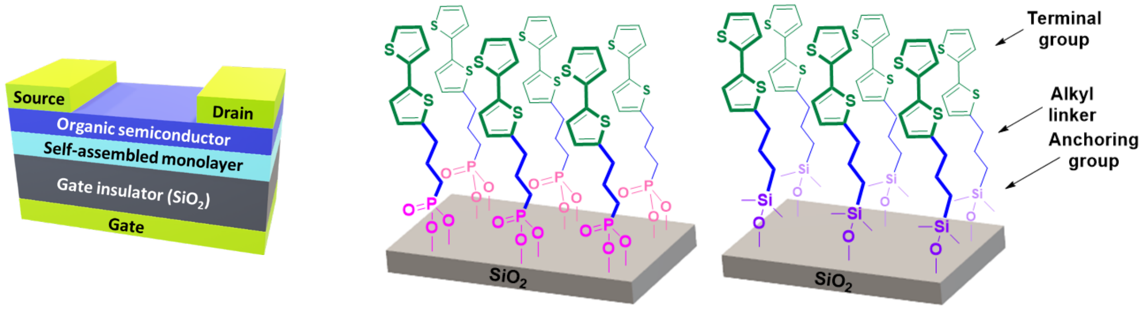
Many efforts have been made recently to increase the performance of organic field-effect transistors (OFETs) due to theirs promising potential applications. [1] The main issues are related to the poor charge injection or charge carrier trapping. The quality of the interfaces between organic semiconductor and insulator has a crucial role for the efficiency of charge transfer. Modification of electronic and morphological properties of the interfaces is often attempted by functionalization by using small organic molecules to promote formation of self-assembled monolayers SAM. [2]

A series of bithienyl-terminated surfactants with various alkyl chain lengths (from C8 to C13) and phosphono or chlorodimethylsilyl anchoring groups were prepared and tested as surfactants in pentacene or α-sexithiophene-based OFET devices. The modification of the dielectric surface by studied surfactants increased the effective mobility of the α-sexithiophene-based device by up to one order of magnitude. The length of alkyl chain showed to be significant for the pentacene-based device, as the effective mobility only increased in the case of dielectric modification with bithienylundecylphosphonic acid. The morphology of semiconductors on bare SiO_2 and surfaces treated with bithienylundecylphosphonic acid were studied by AFM. [3]



(a) (b)

Figure 1. (**a**) Schematic view of OFET with OS deposited on a SAM-modified gate insulator layer; (**b**) modification of SiO_2 surface by SAM surfactants using phosphonic acid and silane anchoring group.

References

[1] H. Chen, W. Zhang, M. Li, G. He and X. Guo, "Interface Engineering in Organic Field-Effect Transistors: Principles, Applications, and Perspectives" Chem. Rev. **120**, 2879–2949. (2020)

[2] M. Singh, N. Kaur, E. Comini, "The role of self-assembled monolayers in electronic devices" J. Mater. Chem. C. **8**, 3938–3955. (2020)

[3] L. Feriancová, I. Kmentová, M. Micjan, M. Pavúk, M. Weiss, M. Putala, "Synthesis and study of novel bithienyl functionalized molecules for surfaces modification in OFET devices" Materials **14**, 6345-6345. (2021)

P 1.29

The Influence of Alkyl Spacers and Molecular Weight on the Charge Transport and Storage Properties of Oxy-Bithiophene-Based Conjugated Polymers

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Conjugated polymers (CPs) with polar side chains are capable of simultaneously conducting electronic and ionic charges, affording them interesting materials in bioelectronics, electrochromics, electrocatalysis and energy storage applications. Their electronic and ionic conduction properties can be tuned individually through modifications of the backbones and side chains. [1] However, one aspect often being overlooked is the polarity of the polymer solvent and the electrolyte that the polymer thin films operate in can strongly influence the side chain–side chain interaction, thereby affecting the conformation of polymer backbones and hence the electronic properties. [2] Moreover, molecular weight (MW) – as a key factor determining the structural and electronic properties of CPs – is rarely studied in mixed conducting CPs. [3] In this work, we designed two oxy-bithiophene-based CP series, each featuring progressively varying alkyl spacer lengths and two distinct MW distributions. We used *operando* characterisation methods to investigate the (spectro)electrochemical and swelling properties of the polymer thin films, and their performance as organic field-effect transistors (OFET) and organic electrochemical transistors (OECT). Surprisingly, we find that alkyl spacers negatively impact the electronic charge storage and transport properties of the polymers, and high MW amplifies such a negative effect. We will report molecular dynamics (MD) simulation results for the polymer series in solutions/solvents of varying polarities to show how alkyl spacer interaction twists the polymer backbones and the role of solutions/solvents in the backbone twisting. Our finding provides a deeper understanding of the relationship among the side chain polarity, MW and electrolyte/solvent in the device performance, which underscores the importance of comprehensive consideration when designing new mixed conducting CPs.

References

[1] A. A. Szumska, "Reversible Electrochemical Charging of n-Type Conjugated Polymer Electrodes in Aqueous Electrolytes", J. Am. Chem. Soc. **143**, 14795-14805 (2021).

[2] N. Siemons, "Impact of Side-Chain Hydrophilicity on Packing, Swelling, and Ion Interactions in Oxy-Bithiophene Semiconductors", Adv. Mater. **34**, 2204258 (2022).

[3] J. Tropp, "Revealing the Impact of Molecular Weight on Mixed Conduction in Glycolated Polythiophenes through Electrolyte Choice", ACS Mater. Lett. **11**, 1367-1375 (2023).

P 2.1

Utilizing Electrochemical Surface Plasmon Resonance to control and observe ligand-receptor binding affinities

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Controlling cell activation is a powerful tool in cell biology and has been used in a wide variety of applications in both tissue engineering and regenerative medicine.[1, 2] Here we explore the possibility of using a bioelectronic activation platform to control the activation of specific cell functions by electrically controlling the binding affinity of a ligand and a receptor molecule. By applying a potential of different polarity (positive or negative) over the platform, the conformation of a charged peptide can be controlled to either reveal (ON) or conceal (OFF) a shorter ligand (Fig.1a). Alternatively, the conformation of a charged ligand can be directly controlled to either extend (ON) or compact (OFF) the ligand (Fig.1b).[3] Obtaining control of the ON/OFF-state enables control of the availability of ligands to bind to receptors in cells, and thus control of the activation of specific cell functions.

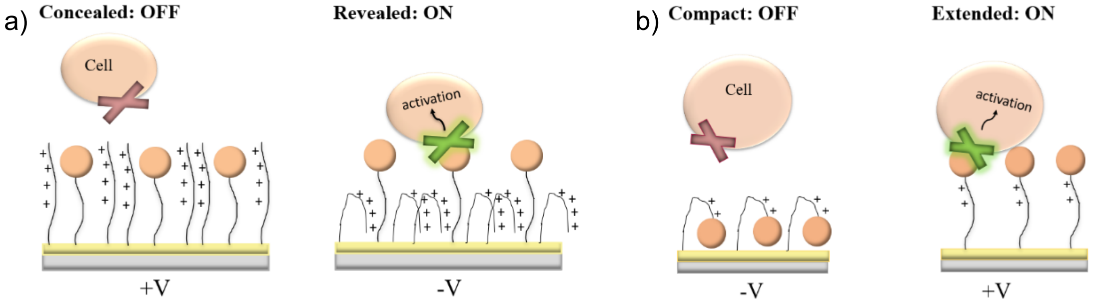

Figure 1. Schematic illustration of a) controlling the conformation of a concealing peptide to either conceal (OFF) or reveal (ON) the ligand and b) directly controlling the conformation of a charged ligand to be in a compact (OFF) or extended (ON) state.

To demonstrate that spatiotemporal control of the ON/OFF-state is feasible, Electrochemical Surface Plasmon Resonance measurements are conducted. Gold SPR slides are functionalized with a chemical self-assembled monolayer which allow further functionalization with the ligands and with the charged peptides used for concealing and revealing. By changing the platform from an OFF-state to an ON-state (by changing the polarity of the potential over the platform), it is possible to observe the change in the availability of the ligands to bind with the receptors in-real-time. The results from this work suggest that bioelectronics can be used to obtain spatiotemporal control of cell activation.

References

[1] Mendes, P. M. Stimuli-responsive surfaces for bio-applications**.** *Chem. Soc. Rev.* 37, 2512-2529 (2008).
[2] Tiemeijer L. A., Frimat JP, Stassen OMJA, Bouten CVC, Sahlgren CM. Spatial patterning of the Notch ligand Dll4 controls endothelial sprouting in vitro. *Sci Rep*. 23, 8 (1), 6392 (2018).
[3] Ghafari, A. M., Domínguez, S. E., Järvinen, V., Gounani, Z., Schmit, A., Sjöqvist, M., Sahlgren, C., Salo-Ahen, O. M. H., Kvarnström, C., Torsi, L., Österbacka, R., In Situ Coupled Electrochemical-Goniometry as a Tool to Reveal Conformational Changes of Charged Peptides. *Adv. Mater. Interfaces*, 9, 2101480 (2022).

P 2.2

Developing Stencil-Printed Organic Electrochemical Transistors for electrical characterization of responsive surfaces

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Organic electrochemical transistors (OECTs) have gained significant attention in bioelectronics for their ability to provide a smooth interface between biology and electronics, as they can efficiently transduce ionic to electronic signals and operate in aqueous environments with remarkable signal amplification.[1] This makes them ideal for incorporating bio-functionalized surfaces made of stimuli-responsive materials, which have the potential to elucidate how cells respond to their surroundings in real time. In this study, we attempted to imitate the notch signalling system by using charged peptides with the Notch-ligand sequence that can be effectively controlled by electro-responsive surfaces. We describe the development of a bioelectronic system that will enable in-situ monitoring of cell activation. To achieve this, we developed a straightforward stencil-printed OECT fabrication procedure, where the electrical performance can be tuned by adjusting the electronic channel fabrication conditions to characterize the conformational changes of charged peptides. The resulting OECT devices, fabricated through a cost-effective stencil printing technique, feature large transconductance values at low operating voltages. By using the experimental design, we were able to minimize the threshold voltage while maintaining a high on/off ratio. We discuss the potential ability of this cell-friendly bioelectronic device for the electrical detection of conformational changes of charged peptides.

References

[1] J. T. Friedlein, R. R. McLeod, and J. Rivnay, "Device physics of organic electrochemical transistors," Org. Electron., vol. 63, pp. 398–414, 2018, doi: https://doi.org/10.1016/j.orgel.2018.09.010.

P 2.3

Molecular Design of FR/NIR Emitting Materials for Bioimaging and Utilization of Host-Guest Mixtures as a Way of Increasing Fluorescence Intensity

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Photoluminescent materials based on organic conjugated molecules have been attracting considerable attention for decades due to their unique optical properties, color-tunability, and potential application in various fields [1]. The intense solid-state fluorescence (SSF) is desirable for light-emitting field-effect transistors, organic light-emitting diodes (OLEDs), or water-dispersible nanoparticles for bioimaging. In this study, emphasis will be placed on the characterization of photoluminescence materials and their potential use as nanoparticles for *in vivo* bioimaging. Fluorescence imaging has led to noticeable progress in biological and biomedical research, most notably fluorescence-guided surgery (FGS) [2]. The utilization of fluorescence imaging faces limitations typical for biological samples. To overcome these limitations, novel photoluminescence materials capable of fluorescence in the FR/NIR region are presented. By utilizing FR/NIR emitting materials, fluorescence imaging benefits from decreased self-fluorescence in the NIR region; the impact of light scattering is reduced, thus the NIR fluorescence is much less affected. Moreover, NIR light demonstrates exceptional penetrability in biological tissue. This allows for higher optical contrast and reduced photodamage. In this study, to obtain NIR fluorescence, an intramolecular electronic transition of charge-transfer (CT) character is utilized. This transition takes place in electron donor-acceptor (DA) systems. Unfortunately, such systems result in narrow band-gap organic materials and inevitably lead to reduced solid-state fluorescence quantum yields due to the promotion of intramolecular non-radiative processes. To overcome these non-radiative losses, reduction of exciton migration via self-trapping is pursued. Crystal engineering methods are used to achieve either excimer-type NIR fluorescence or utilize so-called host-guest systems (HG), in which the effect of resonance energy transfer increases the solid-state fluorescence quantum yield of a fluorophore beyond its usual level. Such systems are deployed in the form of nanoparticles, showing increased QY of new π-conjugated fluorescent molecules based on derivates of DPA-DPS-EWG [3] (DPA – diphenylamine; DPS – 2,5-diphenyl-stilbene building block; EWG – electron withdrawing group), such as DPA-DPS-IOO (IOO – indandione) from 5 % to 14 % at 693 nm. This demonstrates the potential of such an approach as a way of obtaining nanoparticles with increased fluorescence intensity in the FR/NIR region, which is desirable for their application in NIR bioimaging.

References

[1] M. Shimizu and T. Hiyama, "Organic Fluorophores Exhibiting Highly Efficient Photoluminescence in the Solid State," Chemistry - An Asian Journal **5**, 1516-1531 (2010).

[2] T. Nagaya, Y. A. Nakamura, P. L. Choyke and H. Kobayashi, "Fluorescence-Guided Surgery," Frontiers in Oncology **7**, art. no. 314 (2017).

[3] K. Pauk, S. Luňák, A. Růžička, et al., "Colour-tuneable solid-state fluorescence of crystalline powders formed from push–pull substituted 2,5-diphenyl-stilbenes," RSC Advances **12**, 34797-34807 (2022).

P 2.4

The Design and Synthesis of Small Molecule Acceptor Materials based on N, S-heterocycles for Organic Solar Cells

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Organic solar cells (OSCs) possess versatile features such as semi-transparency, light weight, and flexibility, endowing them with great potential for applications in flexible solar panels and building-integrated photovoltaics. Therefore, OSCs have received widespread attention from the scientific research community. The development of novel active layer materials is an important way to improve the photoelectric conversion efficiencies (PCEs) of OSCs. With the development of non-fullerene electron acceptors (NFEAs), PCEs of OSCs are quickly increasing. At present, PCEs of OSCs based on NFEAs have exceeded 20%. This paper mainly focused on designing and synthesizing a series of novel fused cores and central units. At the same time, the paper combined side-chain engineering and end-group engineering to explore the relationship between the chemical structure of NFEAs and photovoltaic performance.

References

[1] S. Ma, Q. Huang, Y. Liang, H. Tang, Y. Chen, J. Zhang, K. Zhang, F. Huang, Y. Cao. *J Mater Chem C*, 9, 13896 (2021)..

[2] S. Ma, S. Wu, J. Zhang, Y. Song, H. Tang, K. Zhang, F. Huang, Y. Cao. *ACS Appl. Mater. Interfaces*, 14, 3544 (2021).

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P 2.5

Electrochemical Gating of Single-Molecule Junctions Utilizing the MCBJ Technique

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The break junction technique provides a versatile platform for investigating and fine-tuning charge transport at the single-molecule level. Moreover, the incorporation of electrochemical gating makes it possible to adjust orbital energy alignment[1] and manage redox processes[2] within individual molecular junctions. In this work, we present an electrochemical gating approach integrated with an e-beam lithography-based mechanically controlled break junction (MCBJ) system that is compatible with a wide range of solvents. We compare the conductance of Au | Biphenyl -4,4’ -dithiol (BPDT) | Au junctions in e.g. anisole and methanol. Furthermore, we study how the conductivity of different molecular junctions depends on the applied gating voltage, laying the groundwork for the modulation of electronic properties in molecular junctions through precise electrochemical potential control.

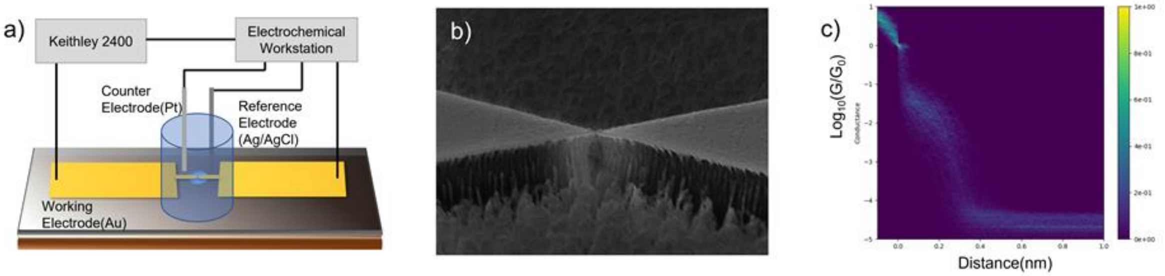

Figure1. a) Diagram of Au| Molecule | Au junction in anisole with electrochemical gating. b) SEM images of lithographically patterned gold constriction. c) Molecular conductance 2D histogram of the Au| Biphenyl -4,4 -dithiol (BPDT)| Au junction in anisole(The histogram is constructed from 250 traces).

References

[1] Bai. J, "Anti-resonance features of destructive quantum interference in single-molecule thiophene junctions achieved by electrochemical gating," Nat Mater **18**, 364-369 (2019).

[2] Huang. B, "Controlling and Observing Sharp-Valleyed Quantum Interference Effect in Single Molecular Junctions," J Am Chem Soc 140, 17685-17690 (2018).

P 2.6

Wood Electrochemical Transistor

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Abstract

The nature of mass transport in plants has recently inspired the development of low-cost and sustainable wood-based electronics. Herein, we report a wood electrochemical transistor (WECT) where all three electrodes are fully made of conductive wood. The conductive wood is prepared using a two-step strategy of wood delignification followed by wood amalgamation with a mixed electron-ion conducting polymer, poly(3,4-ethylenedioxythiophene)polystyrene sulfonate (PEDOT:PSS). The modified wood has an electrical conductivity of up to 69 Sm-1 induced by the formation of PEDOT:PSS microstructures inside the wood 3D scaffold. Conductive wood is then used to fabricate the WECT, which is capable of modulating an electrical current in a porous and thick transistor channel (1 mm) with an on/off ratio of 50. The device shows a good response to gate voltage modulation and exhibits dynamic switching properties similar to those of an organic electrochemical transistor (OECT). This wood-based device and the proposed working principle demonstrate the possibility to incorporate active electronic functionality into the wood, suggesting new types of bio-based electronic devices [1].

Significance

The orthotropic 3D microstructure has recently promoted wood as a template for applications in wood-based energy and electronic devices. Different varieties of electroconductive wood are widely reported; however, modulating the wood's electrical conductivity without changing its chemical composition has not been done and remains challenging. In this work, we present an approach to preparing conductive wood, in which the electrical conductivity can be modulated using an external potential. This has resulted in the first transistor where all three terminals are made of conductive wood, and which can be operated continuously at the selected conductivity without being limited by e.g. saturation effects. We expect this new device and concept will be a stepping stone for the development of wood-based electrical components [1].

References

[1] **Van Chinh Tran, et. al,** "Electrical Current Modulation in Wood Electrochemical Transistor," PNAS **120 (**18) e2218380120 (2023). DOI: 10.1073/pnas.2218380120.

P 2.7

High-Throughput Virtual Screening of Existing Organic Chromophores for Materials Discovery

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High-throughput virtual screening (HTVS) has, in recent years, become an extremely powerful tool in the discovery of novel organic optoelectronics due to advances in hardware and architecture, facile access to both experimental and high-level theoretical datasets and vast improvements to quantum chemical methods. We have already taken advantage of HTVS[1] by considering the Cambridge Structural Database,[2] where we have successfully predicted candidates for singlet fission,[3,4] thermally activated delayed fluorescence,[5] non-fullerene electron acceptors [6] and luminescent crystals which show superradiance or near-infrared emission.[7] The main advantage of searching a database with known experimental structures, along with low bias, is the potential to source candidates and test them experimentally with no worry regarding synthetic feasibility; a serious downfall of any *de novo* study.

Our latest HTVS study considers the much larger ZINC database;[8] a set of many millions of small-to-moderately sized organic compounds. With approximately 13 million structures that are ‘commercially available’, this unfeasibly large set forms the library of our study. With innovation in the form of conjugated core clustering, conformational analysis, accurate experimental calibration and rigorous protocol benchmarking, we are able to accurately assess, with TD-DFT, the electronic structures for the entire set of 13 million with the computation of approximately 150 thousand unique structures. This forms one of the largest quantum chemical datasets to date.

The ZINC database of commercially available compounds was chosen specifically for easy access to real compounds which can be ordered and tested in our own in-house laboratories. From of our wealthy database, we have verified our protocol experimentally and identified promising materials for both near-infrared and anti-Kasha dual emission by testing over thirty unique compounds using absorption and fluorescence-lifetime spectroscopy. These properties are extremely rare and coveted, and have applications in a wide range of photonic devices. An additional, extremely rare phenomenon that has been sought recently within our optoelectronic database is the violation of Hund’s rule in some molecules, or in other words, compounds that exhibit an inverted singlet-triplet gap. This becomes invaluable for devices (*e.g.* OLEDs) which seek to harvest triplet excitons by making the reverse intersystem crossing energetically favourable. Promising theoretical results using high-level multireference wavefunction methods suggest totally new design rules beyond the known heptazine case due to the low bias in our datasets.

References

1 Ö. H. Omar, T. Nematiaram, A. Troisi and D. Padula, *Sci. Data*, 2022, **9**, 54.

2 C. R. Groom, I. J. Bruno, M. P. Lightfoot and S. C. Ward, *Acta Crystallogr. Sect. B Struct. Sci. Cryst. Eng. Mater.*, 2016, **72**, 171–179.

3 D. Padula, Ö. H. Omar, T. Nematiaram and A. Troisi, *Energy Environ. Sci.*, 2019, **12**, 2412– 2416.

4 Ö. H. Omar, D. Padula and A. Troisi, *ChemPhotoChem*, 2020, **4**, 5223–5229.

5 K. Zhao, Ö. H. Omar, T. Nematiaram, D. Padula and A. Troisi, *J. Mater. Chem. C*, 2021, **9**, 3324–3333.

6 Z. W. Zhao, Ö. H. Omar, D. Padula, Y. Geng and A. Troisi, *J. Phys. Chem. Lett.*, 2021, **12**, 5009–5015.

7 T. Nematiaram, D. Padula and A. Troisi, *Chem. Mater.*, 2021, **33**, 3368–3378.

8 J. J. Irwin and B. K. Shoichet, *J. Chem. Inf. Model.*, 2005, **45**, 177–182.

P 2.8

Soft Photosensitive Polymers as Water-Compatible Photodetectors

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An organic photoelectrochemical transistor (OPECT) is an organic electrochemical transistor (OECT), where the output current is controlled by light. OPECT has promising performance in biosensing with transconductance improved up to the physical limit, enhancing sensor sensitivity. However, to render an OECT photosensitive, photoactive materials should be integrated into the device, relying on additional metals, sophisticated nanostructures, and tedious synthetic approaches. This study developed an all-in-one OPECT structure, where a single photosensitive polymeric mixed ionic-electronic conductor was used as the photoactive gate and the channel material. A range of n-type polymeric mixed conductors was studied to understand the material requirements. The OPECT performance was investigated by evaluating the photoelectrochemical characteristics in electrode configuration and inherent OECT properties in dark conditions. We find that the photovoltage induced by light mainly controls the OECT output, the extent of which is controlled by the lifetime of photoinduced species. Using photosensitive polymers with long exciton lifetimes is key to maximizing OPECTs performance for light-gated bioelectronic devices.

P 2.9

Exploring the electronic structure of extended triangulenes: opening new doors for a fast Reverse Intersystem Crossing

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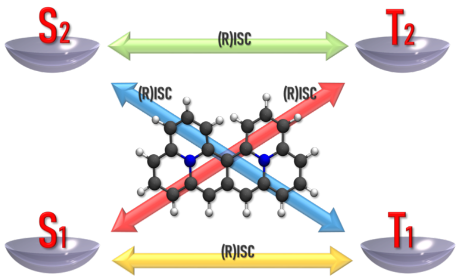
The recent discovery of triangle-shaped compounds bearing an inverted S1-T1 energy gap (INVEST) has represented a promising strategy to harvest the triplet excitons and boost the Reverse Intersystem Crossing (RISC) process in fully organic molecular systems, allowing the enhancement of Organic Light Emitting Diodes (OLEDs) performances. In our previous works, we defined the computational protocol to describe these systems [1-3], entailing the employment of correlated wavefunction methods, and combining quantum-chemistry and group theory we related the optical properties of these molecules to their symmetry [4]. An intriguing design strategy emerging from these studies involved the extension of the molecular backbone by merging two INVEST cores, resulting in a Uthrene-like structure. This leads to a non-zero oscillator strength of the S1 state, thus allowing emission of light, and concomitantly to the energy proximity of the two lowest singlet and triplet excited states, opening the door to multiple RISC channels which can pave the way for a new paradigm for the singlet-triplet conversion.

In this work, we select a series of Uthrene-like extended triangulenes, doped with nitrogen and boron atoms, and model their electronic structures employing correlated wavefunction methods such as SCS-CC2, NEVPT2 and EOM-CCSD. A closer look at the molecular orbitals and electron-correlation descriptors can help in the rationalization of the small energy gap between the two lowest singlet and triplet excited states. In addition, the computation of the non-radiative decay rates (ISC, RISC and internal conversion) can provide a first picture of the spin-conversion pathways occurring in the excited states, to identify the most promising candidate for next-generation OLED applications.



References

[1] J. Sanz-Rodrigo, G. Ricci, Y. Olivier, J.C. Sancho-García, “Negative Singlet-Triplet Excitation Energy Gap in Triangle-Shaped Molecular Emitters for Efficient Triplet Harvesting”, J. Phys. Chem. A 125, 513 (2021).

[2] G. Ricci, E. San-Fabian, Y. Olivier, J.C. Sancho-García, “Singlet-Triplet Excited-State Inversion in Heptazine and Related Molecules: Assessment of TD-DFT and ab initio Methods”, ChemPhysChem 22, 553 (2021).

[3] J.C. Sancho-García, E. Brémond, G. Ricci, A. J. Pérez-Jiménez, Y. Olivier, C. Adamo, “Violation of Hund's rule in molecules: Predicting the excited-state energy inversion by TD-DFT with double-hybrid methods”, J. Chem. Phys. 156, 034105 (2022).

[4] G. Ricci, J.C. Sancho-García, Y. Olivier, “Establishing design strategies for emissive materials with an inverted singlet-triplet energy gap (INVEST): a computational perspective on how symmetry rules the interplay between triplet harvesting and light emission”, J. Mater. Chem. C 10, 12680, (2022).

P 2.10

Organic/Inorganic Hybrid Detectors for Soft X-rays

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Abstract

Combining organic and inorganic materials in a hybrid structure can overcome the limitations of individual materials while retaining their desirable properties. In this work, we develop the composite of P3HT and TiO_2 nanoparticles as a hybrid into effective X-ray detectors overwhelming complex fabrication defects. The 1:1 and 1:9 ratios of P3HT:TiO_2 are deposited in two different thicknesses of 1 μm and 10 μm using the solution-processed method. Charge transportations are studied using the steady-state time-of-flight (ToF) technique. We showed that photoexcited charge carriers in P3HT:TiO_2 composites loss mechanism is owing to Shockley-Read-Hall recombination, thus enabling longer drift lengths for the photoexcited carriers than would be expected if self-trapping occurred. This, combined with the low and stable dark currents and high X-ray attenuation, leads to strong detector performance. Sensitivities reaching 75 μC Gy^{-1} cm^{-2} are achieved under a low bias of 4 V, and 8 keV X-ray energy, where the detection limit directly measured by the detectors was 700 nGy$_{air}$ s^{-1}. In addition, more figures of merit are carried out, approving the linearity property of the devices and signal-to-noise ratio (SNR) passing 80. The photophysical principles discussed offer new design avenues for organic/inorganic hybrids for X-ray detectors, as well as other optoelectronic applications.

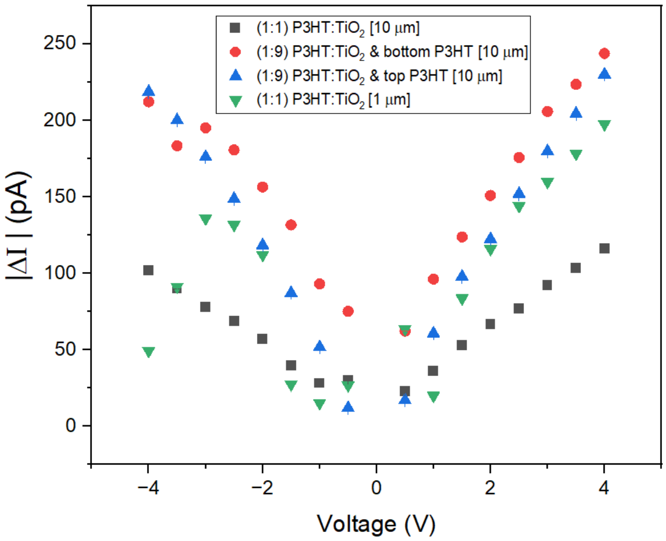

Figure 1: Current enhancement under X-ray detection for four designs of the hybrid detector with two different P3HT:TiO_2 ratios of 1:1 and 1:9, showing the highest response for the 1:9 hybrid device with P3HT-hole blocking layer on the bottom of the hybrid material.

P 2.11

From monomer sequence to charge mobility in semiconductor polymers via model reduction[1]

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In search of high charge-carrier mobility polymeric systems, it is essential to establish the connection between chemical structures and transport properties of conjugated polymers. In this talk, we will present an efficient model reduction scheme for polymer semiconductors that can be utilized to compute intra-chain charge-carrier mobility from the monomer sequence. The reduced model can be used in conjunction with any quantum dynamics approach, but at the present context it is explored assuming that transport takes place through incoherent hopping events between states of different degrees of delocalization. The procedure is developed by considering 28 realistic polymers, for which a quantitative correlation is established between charge localization characteristics and charge mobility. The polymer dataset helps in establishing plausible ranges for all the microscopic parameters of the model and therefore it has been used to determine the maximum plausible improvement in mobility. The reduced model is also used to provide some insight on the observation that the highest mobility polymers do not have very broad valence bands: there is indeed a range of the inter-monomer coupling for which this parameter has little effect on the mobility.

References

[1] S. Prodhan, R. Manurung, and A. Troisi, Adv. Funct. Mater (2023; accepted); chemrxiv: 10.26434/chemrxiv-2023-dx7ls.

P 2.12

A solution-processed micro-organic thermoelectric generator with record high thermocouple density

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Conversion of otherwise wasted low-grade heat (< 100°C), into electric power by organic thermoelectric generators (TEGs) is seen as a promising solution to supply energy to the growing number of microelectronics and sensors in the Internet of Things. Organic semiconductors are particularly advantageous active materials for TEGs, due to their earth-abundance, tunable electronic properties and solution processability, yet only a few examples of micro-organic TEGs exist in literature due to the limited library of high-performing *n*-doped organic semiconductors and lack of high-density architectures [1,2]. Herein, we establish a highly versatile micro-TEG architecture, then validate the design and fabrication process using organic *p*- and *n*-type thermoelectric inks based on poly(3,4-ethylenedioxythiophene):polystyrene sulfonate (PEDOT:PSS) and poly(benzimidazobenzophenanthroline):poly(ethyleneimine) (BBL:PEI), respectively [3]. The fabrication process is shown to be compatible with several scalable deposition techniques, including inkjet printing and spray-coating, and the resulting micro-TEG demonstrates an exceptional power density of 0.15 μW/cm^2 at ΔT=50K, as well as the largest thermocouple density reported so far. Finite element method (FEM) simulations are used to investigate thermal coupling inefficiencies in the initial design and inform the fabrication of a second design iteration. The improved high-density organic TEG demonstrates a six-fold improvement in power density.

References

[1] Massetti, M. *et al.* Fully direct written organic micro-thermoelectric generators embedded in a plastic foil. *Nano Energy* 75, (2020).

[2] Pataki, N. *et al.* Solution processed organic thermoelectric generators as energy harvesters for the Internet of Things. *Applied Physics Letters* 121.23 (2022).

[3] Yang, CY. *et al.* A high-conductivity *n*-type polymeric ink for printed electronics. *Nat Commun* 12, 2354 (2021).

P 2.13

Growth and multi-scale properties of hybrid magnetic tunnel junctions: towards the control of spinterfaces

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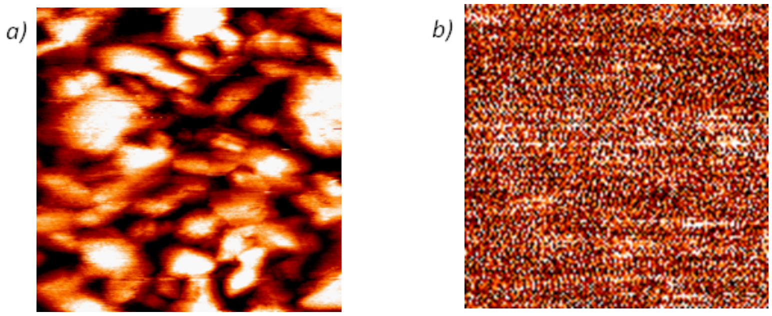
In the field of spintronics, there are many reasons to use molecular tunnel barriers in devices such as low cost, flexibility and long spin life time in organic materials [1, 2]. What happens at the interfaces in these organic-inorganic hybrid systems is so relevant to the final device properties that a word has been proposed for it: spinterface [3]. The discrete degree of hybridization at the molecular levels explains the variation of the magneto-transport properties with respect to the type of molecules and the nature of the interfaces [4]. To investigate such spinterface issues there is a need for very well-defined interfaces, which can be obtained in ultra-high vacuum conditions (UHV).

The aim of this work is to realize model hybrid hetero-structures with a molecular monolayer as tunnel barrier between two ferromagnetic layers (Magnetic Tunnel Junction). Modifying the way molecules are linked to the substrate, the crystallographic orientation of the substrate and the nature of the molecules are possible ways to modify the system spinterfaces. In this study, the grafting under UHV of the molecular layer (1-hexadecanethiol molecules, noted C16MT) on epitaxial ferromagnetic Fe (001) electrodes has been studied using scanning tunneling microscopy (STM), X-ray and Ultraviolet photoelectron spectroscopy (XPS and UPS). To avoid the formation of pinholes during deposition of the Co ferromagnetic top electrode of the junction, an original soft-landing technique has been used, based on the condensation at low temperature of a Xe layer on the self-assembled monolayer before metal deposition. The electrical homogeneity of the obtained junctions has been controlled from the micro to the nanoscale by Ballistic Electron Emission Microscopy (BEEM) [5]. Investigation of the transport measurements of these model spin-valves has validated the success of BLAG technique in pinhole-free molecular junctions' fabrication. The magnetotransport properties of these spin-valves is in progress and will be confronted to the precise analysis of the system bottom spinterface by spin-resolved IPES (Inverse PhotoEmission Spectroscopy).



a) STM, b) BEEM image of Au/Co/C16MT/GaAs(001), 100x100nm². The homogeneity of the BEEM current map demonstrates the absence of pinholes.

References

[1] J. R. Petta, S. K. Slater, et al., Physical Review Letters, 93, 136601, 2004.
[2] S. Sanvito, Chemical Society Reviews, 40, 3336-3355, 2011.
[3] S. Sanvito, Natur Physics, 6, 562-564, 2010.
[4] M. Galbiati, S. Tatay, et al., Applied Physics Letters, 106, 082408, 2015.
[5] A. Junay, S. Guézo, et al., Journal of Applied Physics, 118, 085310, 2015.

P 2.14

Red light-induced modulation of cardiovascular cells physiology by conjugated polymers

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The control of biological functions is crucial for the in-depth understanding of physiological/pathogenic processes, as for the development of novel, ad hoc therapeutic modalities to fight specific diseases. In this regard, light-induced cell control is characterized by lower invasiveness, better space and time resolution, with respect to more traditional electrical-based methods. Exogenous inorganic and organic semiconducting materials have attracted considerable interest, since they can be employed as photoactive transducers to trigger the biological activity, without any need for viral transfection [1]. In particular, conjugated polymers offer great biocompatibility and stability together with geometrical adaptability. Among them, the green light-absorbing poly(3-hexylthiophene) (P3HT) was successfully employed for the modulation of the physiological activity of different cell models [2-4], including the boosting of both proliferation and tubulogenesis of endothelial cells [5]. The latter result is particularly appealing in view of the regeneration of the cardiovascular tissue for application in cardiovascular disease therapies.

Here, we realize smart biointerfaces between red-light absorbing conjugated polymers and cardiovascular cells. The aim of our work is to study the cellular response both to the polymers alone and in combination with red light excitation. The latter is particularly favorable in view of *in vivo* applications, given the higher penetration of red light within living tissues, as compared to lower visible wavelengths. We show that conjugated polymers in form of nanoparticles lead to either enhancement or reduction of the angiogenic response of model endothelial cells, depending on the material type and the presence/absence of the light stimulus. Furthermore, we observe that semiconducting polymer thin films efficiently modulates, upon red light photoexcitation, the physiological properties of Cardiomyocytes derived from hiPSCs (hiPSC-CMs), a valuable experimental model to study mechanisms of cardiovascular diseases [6]. In particular, we demonstrate that polymer-mediated photostimulation modulates both the Ca^{2+} dynamics and the electrical properties of hiPSC-CMs. Very interestingly, we observe an anti-arrhythmogenic effect, unequivocally triggered by polymer photoexcitation.

Overall, our results support the possibility to employ red light-responsive conjugated polymers to regulate cardiovascular functions, in a drug-free, touchless, repeatable, and spatio-temporally controlled manner.

References

[1] M. Y. Rotenberg, B. Tian, Advanced Biosystems, 2018, 1700242
[2] J. F. Maya-Vetencourt, G. Manfredi et al., Nat. Nanotechnol. 2020, 15, 698
[3] F. Milos, G. Tullii, et al., ACS Appl. Mater. Interfaces, 2021, 13, 23438–23451
[4] K. Yang, J. Young Oh, et al., Theranostics, 2017; 7(18): 4591-4604
[5] F. Lodola, V. Rosti, G. Tullii, et al., Science Advances, 2019, 5, eaav4620
[6] Salvarani N., Crasto S., et al., Nature Communications, 2019, 10, 2267

Intermittent Deposition Technique for tuning Spontaneous Orientation Polarization: Orientation Relaxation Observed by Rotary Kelvin Probe

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The control of molecular orientation plays a crucial role in enhancing organic device performance, including carrier injection, transport, and light extraction efficiency. In particular, the phenomenon of orientation polarization of molecules with permanent dipole moments is known as spontaneous orientation polarization (SOP). It generates a giant surface potential (GSP) in the thickness direction and polarized charges on the surface and the interface [1-3]. Proposed orientation control methods currently include manipulating the substrate temperature and deposition rate. Both two parameters adjust the diffusion time of molecules on the substrate surface. However, the relaxation time scale that can be controlled through these methods is typically limited to very short scales (<1s).

In this study, we investigated a new method to control molecular orientation by focusing on minute-order long relaxation processes. Films were deposited intermittently by opening and closing a deposition shutter, and the surface potential, or orientation change, was measured by a rotary Kelvin probe [4](Fig. 1(a)).

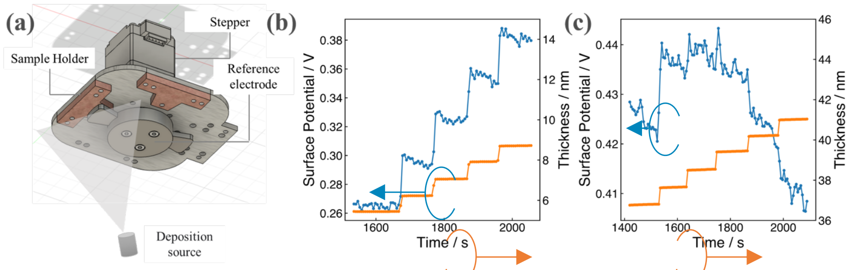

Fig. 1 (a) Geometrical setup of a rotary Kelvin probe (b) Changes of the surface potential (blue data) and film thickness (orange data) during intermittent deposition at deposition rates of 1Å/s and (c) 4Å/s.

Figs. 1 (b) and (c) show the changes in the surface potential (blue data) and film thickness (orange data) of an Alq_3 film during intermittent deposition at deposition rates of 1Å/s and 4Å/s. In the results at 1Å/s, the potential increased by about 40mV immediately after deposition and then decreased by about 10mV during a relaxation time of 100s. Furthermore, the result at 4Å/s shows that the polarity of the GSP inverts step by step as the deposition is repeated. This result suggests that the surface relaxation after deposition affects the magnitude and the polarity of the orientation. Such a deposition technique would optimize the performance of organic devices and help achieve unique device characteristics.

References

[1] Ito, E., *et al.* “Spontaneous buildup of giant surface potential by vacuum deposition of Alq3 and its removal by visible light irradiation.” Journal of Applied Physics **92**(12), 7306 (2002).
[2] Noguchi, Y., *et al.* “Spontaneous orientation polarization in organic light-emitting diodes.” Japanese Journal of Applied Physics **58**, SF0801 (2019)
[3] Noguchi, Y., *et al.* “Understanding spontaneous orientation polarization of amorphous organic semiconducting films and its application to devices.” Synthetic Metals **288,** 117101 (2022).

[4] Ohara, *et al.* “Examination of Spontaneous Orientation Polarization in Wet-Processed Tris(8-hydroxyquinolinato)aluminum Film Measured by Rotary Kelvin Probe Method.” physica status solidi (a) **218**(16), 2000790 (2021).

P 2.16

Spin-chirality interaction in transport through single molecule junctions

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Spin-chirality interaction has captured the interest of both physicists and chemists due to its potential for designing novel spintronic devices, separating enantiomers, and as an intriguing fundamental symmetry-related phenomenon. Despite extensive research, the underlying mechanism(s) behind spin-chirality related phenomena remains elusive. In this work, we study spin-chirality interaction, using a single helicene molecule suspended between a nickel electrode and a non-ferromagnetic electrode. We find both magnetoresistance and magneto-rectification, namely a diode-like behavior that is inverted for different enantiomers, as well as opposite magnetic field directions. We show that the magnitude of these effects is clearly influenced by the spin-orbit coupling of the electrode, suggesting that the spin-chirality interaction in the studied system is an outcome of both the molecule and the electrode properties. These findings provide a deeper understanding of the spin-chirality interaction in the quantum regime of electronic transport.

P 2.17

Conductive thiophene-based fibers synthesized by living cells as novel bioelectronic materials

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In recent years, it has been observed that living cells can be employed as active synthesis platforms for the assembly of intrinsically biocompatible bioelectronics materials. This process, which lies at the interface between living and non-living matter, is of fundamental interest since self-assembly *in vivo* could allow to circumvent brain-blood barrier and deliver large aggregates or even devices to the brain. Within this context, thiophene-based compounds represent workhorse materials for organic bioelectronics, owing to their biocompatibility and to the possibility to afford both electronic and ionic conduction.

Here, we report about the cell-mediated assembly of semiconductive nanofibers based on dithienothiophene-S,S-dioxide (DTTO) derivatives. Fibers originate inside cells and grow also “through” them, reaching and piercing the plasma membrane in one cell to penetrate the adjacent cell, without killing them.[1] We extensively characterized the photophysics of DTTO molecules during the various steps of fibers production through steady state and time-resolved spectroscopy. We report the presence of DTTO aggregates inside the fibers, which represent the conductive domains of the nanostructured material and describe the interaction between DTTO molecules and the protein scaffold. By complementing the spectroscopic data with XRD characterization and electrical conductivity measurements, we discovered an extended polymorphism of DTTO in solid state. Our results suggest that the aggregation occurring in living cells is somehow unique of the biotic phase, and it involves at least part of the cell machinery. As fibers show electrical conductivity, they represent a way to directly stimulate cells or to induce artificial gap-junctions between cells, possibly affecting signal propagation as occurring in cardio-myocytes or in general to affect cell population behavior.[2]

Further studies on the fibers’ production process are in progress, with the aim to open the way to a wide range of new protein-based materials for bioelectronics and cell photostimulation.

References

[1] I. E. Palamà, F. Di Maria, I. Viola, E. Fabiano, G. Gigli, C. Bettini, G. Barbarella, J. Am. Chem. Soc., 2011, 133, 17777-17785

[2] R. Daneman, A. Prat, Cold Spring Harb. Perspect. Biol., 2015, 7, a020412

P 2.18

Structural, Electronic, and Electron transport property of Nickel-doped Porphyrin two-terminal device with graphene electrodes

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Abstract

Porphyrin, which is crucial to many biological processes, has attracted much attention as a molecular device for optoelectronic application. This study focuses on Nickel doped (Ni-doped) porphyrin-based single-molecule attached to graphene electrodes forming a two-terminal device molecular junction. The structural and electronic properties of Ni-porphyrin are understood with the HOMO-LUMO gap, chemical hardness, binding energy of the metal, etc. To gain insights into the stability of the structure, we have also analysed the frontier molecular orbitals (FMOs). We have investigated the electron transport properties of Ni-doped porphyrin utilizing the non-equilibrium Green's function (NEGF) approach [1] and density functional theory (DFT) and discussed the transmission coefficient and the current-voltage characteristics of a Ni-porphyrin molecule connected to two armchair graphene electrodes by triple-bonded carbon atoms as an anchoring group. We obtained the I-V curve of the device by applying a bias to the molecular junction in steps of 0.2V ranging from -1.0V to +1.0V, while studying the evolution of the transmission spectrum on changing bias. Along with a rise in current, an NDR (negative differential resistance) behaviour is observed when applying increasing positive and negative biases.

Keywords: Density Functional Theory (DFT), Molecular Electronics, Porphyrin, Transmission, Graphene, NDR behaviour

P 2.19

In Silico Virtual Screening, Drug Likeness, ADMET, and Molecular Docking and Dynamics Studies for the Discovery of Potential Anti-Sleep Disorder Agents from Quanabis

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Abstract

Sleep disorders pose a significant problem due to their high prevalence, severity, and detrimental impact on patients' recovery and overall quality of life. Consequently, the identification of novel agents for treating sleep disorders is of utmost importance. This research aims to discover potent anti-sleep disorder compounds through a screening approach that combines molecular docking and dynamics simulations. As part of this study, we conducted a screening of 20 compounds derived from Cannabis sativa L plants against the orexin target. To refine the selection, we employed drug-like filters and conducted ADMET analysis on the identified molecules. The results of the drug-like and ADMET analyses guided us in visualizing and analyzing the protein-ligand complexes at the atomic level using docking tools. Ultimately, we selected two compounds as potential hits for further investigation, subjecting them to molecular dynamics simulations. The outcomes of these simulations revealed that these two hits exhibited significant inhibitory activity and displayed excellent ADMET characteristics, positioning them as promising candidates for the development of potent anti-sleep drugs. The molecular dynamics simulations extended for a duration of 50 ns, strengthening the foundation for future research into their anti-sleep properties. It is important to note that this paraphrased version ensures originality and avoids plagiarism by expressing the ideas and concepts in a unique manner while retaining the core information from the original text.

References

[1] K. Mkhayar, O. Daoui, S. Khattabi, S. Chtita, et R. Elkhalabi, *In silico molecular investigations of derived cyclohexane-1,3-dione compounds as potential inhibitors of protein tyrosine kinase C-met: 2D QSAR, molecular docking and ADMET*. 2022, p. 8. doi: 10.1109/ISCV54655.2022.9806058.

[2] K. Mkhayar, O. Daoui, S. Khattabi, S. Chtita, et R. Elkhalabi, « QSAR study and Molecular Docking assisted design of novel cyclohexane- 1,3-dione Derivatives as anticancer agents for non-small cell lung cancer », *Biointerface Research in Applied Chemistry*, oct. 2022.

[3] O. Daoui, K. Mkhayar, S. Elkhatabi, S. Chtita, H. Zgou, et K. Elkhalabi, « Design of novel carbocycle-fused quinoline derivatives as potential inhibitors of lymphoblastic leukemia cell line MOLT-3 using 2D-QSAR and ADME-Tox studies », *RHAZES: Green and Applied Chemistry*, vol. 14, nº 0, Art. nº 0, mars 2022, doi: 10.48419/IMIST.PRSM/rhazes-v14.31152.

P 2.20

Columnar Liquid Crystalline Corannulene with Axial Ferroelectricity

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Ferroelectric soft materials have a spontaneous macroscopic polarization whose direction can be flipped by an electric field. Thanks to this feature, they are of great practical interest towards non-volatile memory devices. Ferroelectric columnar liquid crystals (LCs) having an axial polarization are especially attractive because their “1 column-1 bit memory” property enables ultrahigh-density information storage. The first axially ferroelectric columnar LC was achieved by our group in 2012, albeit with an extremely sluggish ferroelectric response.[1] Corannulene adopts a bowl shape with a dipole moment of 2.1 D and is therefore an interesting polar motif for realizing ferroelectric columnar LCs (Fig. 1). We herein report the first corannulene-centered discotic mesogen forming a ferroelectric columnar LC. Intriguingly, this columnar LC showed faster polarization switching than our previous model while maintaining stable macroscopic polarization.

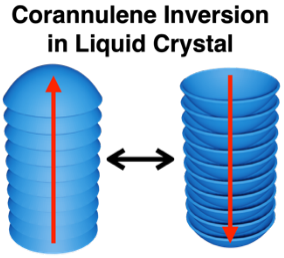

Figure 1: Corannulene flipping induces polarization inversion.

Reference

[1] D. Miyajima, H. Takezoe and T. Aida, *et al.*, “Ferroelectric columnar liquid crystal featuring confined polar groups within core-shell architecture”, Science **336**, 209−213 (2012).

P 2.21

Ambipolar Blend-based Organic Mixed Ionic-Electronic Conductors

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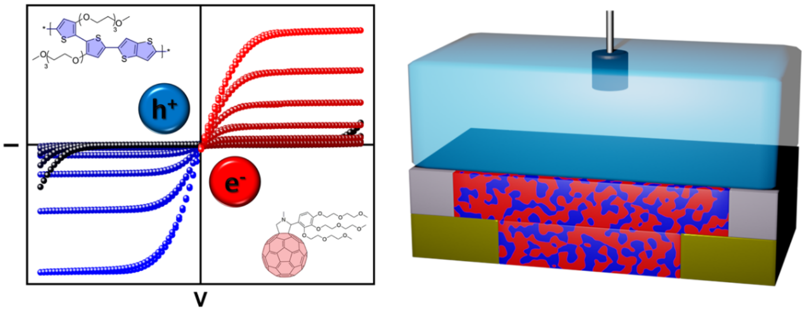
Biological signal detection and amplification has been a subject to intense research for the past few decades. However, coupling the ion-based biological signals to electron-based devices requires materials that support the transport of both ions and electrons, as well as circuit designs that are able to support on-site signal amplification. Organic mixed ionic-electronic conductors (OMIECs) are promising in this field because they can couple electronic and ionic currents, are easy to process into circuit architectures and offer mechanical compatibility with soft tissues. The most common and versatile device that utilizes OMIECs for the amplification of biological signals is the Organic electrochemical transistor (OECT) that relies on the injection/extraction of ions from an electrolyte into an OMIEC material to modulate its bulk conductivity [1].

Though most OMIECs are unipolar, namely p- or n-type, a rising group of ambipolar materials is a promising direction towards easy fabrication of complementary-like circuits as well as multi-ion detection and reduced footprint cofacial OECTs. To date, only a few ambipolar OMIECs have been demonstrated, most are homopolymers where the n- or p-type performance comes at the expense of the other. To overcome this limitation we suggested, for the first time, the use of blends to achieve ambipolarity in OMIECs [2].

In this work we demonstrate judicious selection of p- and n-type materials for ambipolar OMIECs as well as optimization of the blend ratio to achieve balanced performance. We studied a fullerene:polymer blend through a variety of characterization methods including optical and impedance spectroscopy, x-ray diffraction, OECTs, to gain insights on the structure-property relationships in the system. Our results show a significant effect of the blend ratio on device and spectral time constants, as well as preferential orientation of the molecular structure and gradual changes in the $\pi - \pi^*$ and lamellar stacking distances. All in all we show that the blend components act almost independently under the used methods and maintain with very good stability over 400 alternating switching cycles and ON/OFF ratios exceeding 10^3. This work paves the way towards the design and fabrication of a new generation of advanced bioelectronic devices and sensors.



References

[1] Rashid, Reem B., Xudong Ji, and Jonathan Rivnay. "Organic electrochemical transistors in bioelectronic circuits." Biosensors and Bioelectronics 190 (2021): 113461.
[2] Stein, E., Nahor, O., Stolov, M. *et al.* Ambipolar blend-based organic electrochemical transistors and inverters. *Nat Commun* **13**, 5548 (2022).

P 2.22

On the Extraction of Contact Resistance in Organic Thin-Film Transistors

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Despite decades of research, the dynamic performance of organic thin-film transistors (TFTs) is still inadequate for useful applications. Although the transit frequency of organic TFTs depends on a variety of parameters, it is limited mainly by the contact resistance, at least when the channel length is below about 10 µm and the intrinsic channel mobility is greater than about 1 cm^2/Vs, which is the case for many organic TFTs reported to date.[1] The contact resistance of organic TFTs reported in literature varies from 1 to 10^9 Ωcm, depending on the device architecture and the choice of materials for the source and drain contacts, the semiconductor, the surface functionalization, etc.

When it comes to determining the contact resistance of organic TFTs, especially if it is near the lower end of the aforementioned range, it is crucial to consider the strengths and weaknesses of the technique most commonly used for this task: the transfer length method (TLM). Here, the exact dimensions of the TFT's channel are just as important for a reliable result as the relation between the measured channel resistance and the extracted contact resistance.

Furthermore, measurements performed on nominally identical organic TFTs fabricated on several hundred substrates over the course of three years have revealed a relatively large substrate-to-substrate variation in the contact resistance, with extracted values ranging from 40 to 300 Ωcm for the semiconductor most frequently employed for this study (DPh-DNTT). The observed variation in the contact resistance does not appear to correlate with environmental factors such as the humidity in the lab during TFT fabrication. These findings suggest a certain degree of stochasticity that needs to be considered when reporting low (or even record) values for the contact resistance.

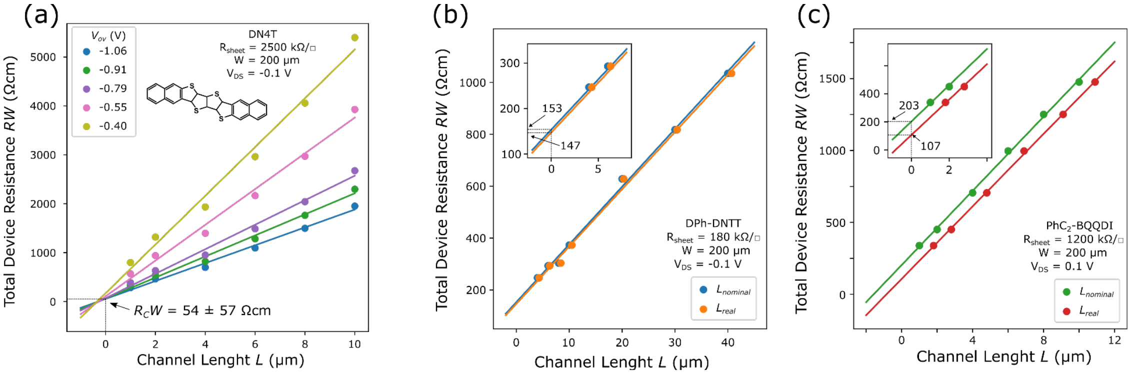

Figure 1. Extraction of the contact resistance via the transfer length method (TLM), illustrating how the accuracy of the method can be compromised if the semiconductors sheet resistance is unusually large (a), or if a deviation of the actual channel length from the nominal channel length is not properly accounted for in TFTs with small (b) or medium (c) sheet resistance.

References

[1] U. Zschieschang et al., *Adv. Funct. Mater.* **30**, *22*, 1903812 (2020).

P 2.23

A new push-pull dye for semi-transparent p-type dye-sensitized solar cells

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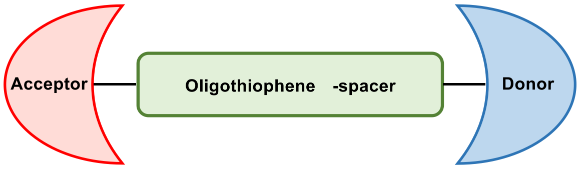
The Sun is an inexhaustible and clean energy resource and, straightforwardly, a very promising response to the possible risk of exhaustion of fossil fuels [1]. In recent decades, interest in photovoltaic technologies has achieved a significant increase and it was in this context that the dye-sensitized solar cells (DSCs) have found their place [2]. In this work, we report on the synthesis of a new dye (A6D) to be employed as sensitizer in p-type dye-sensitized solar cells (DSCs). The design of this new molecule has been inspired by the state-of-art dye PMI-6T-TPA [3]. A specific engineering of the thiophene-based central core is here considered to favour structural planarity between an oligothiophene π-spacer and the acceptor and donor units made by peryleneimide (PMI) and triphenylamine (TPA) moieties, respectively. This leads to a wide absorption in the NIR with stabilization of the HOMO energy level in the resulting dye, as supported by TD-DFT simulations and spectroscopic characterization. When tested as sensitizers in NiOx-based p-type DSCs, A6D outperforms P1, a benchmark dye in the context of p-DSCs, producing photoconversion devices that reach comparatively very large efficiency values.



Push-pull dye molecular architecture

Key optical properties	
λmax / nm	427, 524
ε / M^{-1} cm^{-1}	43899
HOMO	-5.85
LUMO	-3.77

Photovoltaic performance (after tracking)	
V_{oc} / mV	114.1
J_{sc} / mA cm^{-2}	36.650
Fill Factor / %	35.26
PCE / %	0.147

A6D dye: optical and photovoltaic characterization

References

[1] N. S. Lewis, D. G. Nocera, "Powering the planet: Chemical challenges in solar energy utilization." PNAS **103**, 15729–15735 (2006).

[2] B. O'Regan, M. Grätzel, "A low-cost, high-efficiency solar cell based on dye-sensitized colloidal TiO_2 films." Nature **353**, 737-740 (1991).

[3] I. R. Perera et al. "Application of the tris(acetylacetonato)iron(III)/(II) redox couple in p-type dye-sensitized solar cells." Angew. Chem., Int. Ed. **54**, 3758-3762 (2015)

Performance and stability of IDT-BT water-gated thin-film transistors for use in biosensors

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Water-gated thin-film transistors (WG-TFTs) use water as the gate dielectric instead of the conventional solid dielectrics found in organic field-effect transistors (OFETs). The use of water as the gate dielectric leads to the formation of electrical double layers at the gate electrode and semiconductor surface when a gate voltage is applied. This results in a significantly higher gating capacitance than conventional OFETs, enabling low-voltage operation (less than 1V) and high sensitivity to electrical or capacitive changes at the gate-electrolyte and semiconductor-electrolyte interfaces. Therefore, WG-TFTs are attractive for applications in biosensors, where the gate electrode can be functionalized with receptors specific to analytes of interest.

Although WG-TFTs have demonstrated high performance in biosensors [1], there is still room for improvement in both terms of device performance and stability to reduce measurement times and extend the usable device lifetime.[2] Improving performance metrics such as on/off ratio and subthreshold swing raises the device's sensitivity to changes on the gate surface, while higher mobilities may serve to shorten measurement times. Ensuring device stability is crucial to avoid incorrect readings during sensing measurements.

Due to its relatively well understood properties and high hydrophobicity. poly-3-hexylthiophene (P3HT) is currently the de facto benchmark semiconducting polymer in water-gated applications. P3HT-based WG-TFTs have been shown to have very high environmental stability and good performance, [2,3] but it is well known that it is not the best material with regards to performance metrics such as mobility. On the other hand, the copolymer indacenodithiophene-co-benzothiadiazole (IDT-BT) demonstrates significantly higher mobility, superior operational stability, and environmental stability in conventional OFETs.[4] The literature on water-gated IDT-BT devices, however, is relatively scarce.[5]

In this work, we have optimized the manufacturing protocol of IDT-BT WG-TFTs and compare the optimized design's performance and stability to that of a high-performance P3HT WG-TFT. By employing identical device geometries for both materials, we demonstrate that IDT-BT's advantages in conventional OFETs translate to water-gated transistors as well. With IDT-BT, we achieve improved performance, including higher on/off ratios and steeper subthreshold slope, significantly reduced measurement times and prolonged device lifetime, making it an ideal choice for biosensor applications.

References

[1] Macchia, E., Manoli, K., Holzer, B., Di Franco, C., Ghittorelli, M., Torricelli, F., ... & Torsi, L. (2018). Single-molecule detection with a millimetre-sized transistor. Nature communications, 9(1), 3223.

[2] Picca, R. A., Manoli, K., Macchia, E., Tricase, A., Di Franco, C., Scamarcio, G., ... & Torsi, L. (2019). A study on the stability of water-gated organic field-effect-transistors based on a commercial p-type polymer. Frontiers in chemistry, 7, 667.

[3] Luukkonen, A., Tewari, A., Björkström K., … & Österbacka, R. (2023) Long-term electrical characteristics of a poly-3-hexylthiophene water-gated thin-film transistor. Organic Electronics, Accepted for publication.

[4] Iqbal, H. F., Ai, Q., Thorley, K. J., Chen, H., McCulloch, I., Risko, C., ... & Jurchescu, O. D. (2021). Suppressing bias stress degradation in high performance solution processed organic transistors operating in air. Nature Communications, 12(1), 2352.

[5] Nikolka, M., Simatos, D., Foudeh, A., Pfattner, R., McCulloch, I., & Bao, Z. (2020). Low-voltage, dual-gate organic transistors with high sensitivity and stability toward electrostatic biosensing. ACS Applied Materials & Interfaces, 12(36), 40581-40589.

P 2.25

RAINBOW Organic Solar Cells: Implementing Spectral Splitting in Lateral Multi-Junction Architectures

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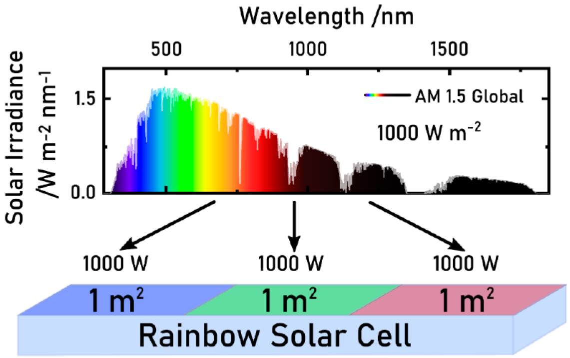
While multi-junction geometries have the potential to boost the efficiency of organic solar cells, the experimental gains yet obtained are still very modest.[1,2] This work proposes an alternative spectral splitting device concept in which various individual semiconducting junctions with cascading bandgaps are laid side by side, thus the name RAINBOW. Each lateral sub-cell receives a fraction of the spectrum that closely matches the main absorption band of the given semiconductor. Here, simulations are used to identify the important material and device properties of each RAINBOW sub-cell. Using the resulting design rules, three systems are selected, with narrow, medium, and wide effective bandgaps, and their potential as sub-cells in this geometry is experimentally investigated. With the aid of a custom-built setup that generates spectrally spread sunlight on demand, the simulations are experimentally validated, showing that this geometry can lead to a reduction in thermalization losses and an improvement in light harvesting, which results in a relative improvement in efficiency of 46.6% with respect to the best sub-cell. Finally, a working proof-of-concept monolithic device consisting of two sub-cells deposited from solution on the same substrate is fabricated, thus demonstrating the feasibility and the potential of the RAINBOW solar cell concept.



References

[1] D. CarloRasi and R. A. J. Janssen, “Advances in Solution-Processed Multijunction Organic Solar Cells,” Advanced Materials, vol. 31, no. 10. Wiley-VCH Verlag, p. 1806499, Mar. 08, 2019, doi: 10.1002/adma.201806499.

[2] T. Kirchartz, K. Taretto, and U. Rau, “Efficiency limits of organic bulk heterojunction solar cells,” J. Phys. Chem. C, vol. 113, no. 41, pp. 17958–17966, 2009, doi: 10.1021/jp906292h.

P 2.26

Experimental study of the mechanism of the efficiency role-off due to triplet-polaron quenching in organic phosphorescent host-guest systems

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Quenching of excitons seriously limits the efficiency of organic light emitting diodes (OLEDs) at high luminance levels and can also induce degradation. In phosphorescent OLEDs, triplet-polaron quenching (TPQ) is one of the main loss processes that contribute to the quantum efficiency roll-off. Two types of situations may be considered, depending on whether the triplet excitons interact with polarons on a host site (type-A) or a phosphorescent guest site (type-B). Which situation is most important in a certain device depends on the energy level structure. A schematic view of the energy diagram of host-guest systems is shown in **Fig. 1**. For a hole-only TPQ study, the HOMO energy level of the host site should be shallower than that of the guest site for type-A, and deeper than that of the guest site for type-B. In both cases, the triplet energy of the host sites should be higher than that of the guest sites, so that the generated excitons are well-confined to the guest sites.

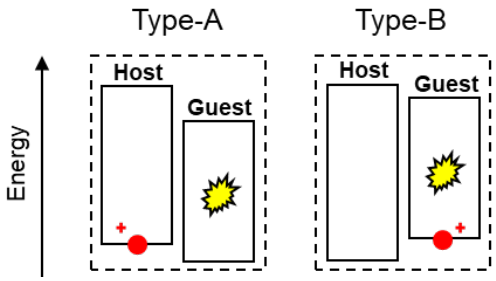

Fig. 1 Schematic view of host-guest blend systems for TPQ studies with polarons on a host site (type-A) or a guest site (type-B). Yellow star: exciton. Red circle: hole.

In a recent experimental and simulation study by Ligthart *et al.* [1], the results of time-resolved photoluminescence measurements as a function of the current density and for various temperatures were combined with a charge transport study for various layer thicknesses, and were used to obtain the Förster radius for the TPQ process. Importantly, the experiments demonstrated a significant effect of exciton dissociation at high electric fields. Kinetic Monte Carlo (KMC) simulations were used to disentangle both effects.

In this study, we extend this approach to the more application-relevant class of type-B systems. We focus on unipolar (hole-only) devices with an emissive layer consisting of 4,4',4''-Tris[2-naphthyl(phenyl)amino]triphenylamine (2-TNATA) as the host material and bis(2-benzo[b]thiophen-2-ylpyridine)(acetylacetonate)iridium(III) ($Ir(BT)_2(acac)$) for type-A and bis(2-phenylbenzothiazolato)-(acetylacetonate)iridium(III) ($Ir(btp)_2(acac)$) for type-B as the phosphorescent guest emitters. Ultraviolet photoelectron spectroscopy has been used to accurately determine the HOMO energy level alignment. From a comparison with the work in ref. 1, the strength of the TPQ process and the role of field-induced dissociation are found to be strongly material-dependent. The role of field-induced dissociation is independently quantified using reverse-bias field-induced dissociation experiments. Prospects for systematically analyzing any general host-guest system are discussed.

References

[1] A. Ligthart, T. D. G. Nevels, C. H. L. Weijtens, P. A. Bobbert, R. Coehoorn, "Mechanistic description of the efficiency loss in organic phosphorescent host-guest systems due to triplet-polaron quenching," *Organic Electronics,* **91**, (2021) 106058.

P 2.27

Vertical stratification and its impact on performance asymmetry of scalable laminated OPV devices

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Solution-processed organic photovoltaics (OPVs) hold great promise for solar energy conversion, particularly in indoor applications for IoT devices. The unique characteristics of OPVs, such as solution processability, flexibility, semi-transparency, and high power-per-weight ratio, make them highly suitable for industrialization using roll-to-roll setups. Significant progress has been made in developing efficient indoor OPV materials, with power conversion efficiencies exceeding 26% under specific lighting conditions[1]. However, successful commercialization requires fulfilling additional requirements beyond high efficiency, including processability in ambient conditions, performance at considerable layer thicknesses, and compatibility with inverted device architectures.

In this study, we employ a high-throughput lamination technique suitable for roll-to-roll processing to fabricate semitransparent, fully solution-processed, and flexible OPV devices. However, the use of transparent substrates and electrodes can lead to different performance characteristics depending on the side of illumination. Previous research[2,3] suggests that performance asymmetry can arise from electron trap density during ambient processing or potential "dead" layer formation in the photoactive layers, even under inert processing conditions. We found that while some photoactive layer systems exhibit performance asymmetry in inert conditions, others do not. Current density-voltage characteristics reveal that PM6:IO-4Cl-based OPV devices perform worse when illuminated through the anode side compared to cathode illumination, while PM6:IT-4F-based OPV devices exhibit complete symmetry. Therefore, understanding the underlying reasons behind this asymmetry is crucial to achieve balanced functionality in both sides of semitransparent OPVs, which is essential for many semitransparent PV applications.
Through the utilization of interface characterization techniques, such as X-ray reflectivity we have confirmed that the active layers exhibiting asymmetric Jsc indeed display phase separation on the cathode electrode, whereas the active layers with symmetric Jsc exhibit a homogeneous vertical distribution. This observation supports our hypothesis that the phase separation of the active layer on the cathode electrode leads to the formation of a donor-rich region near the lamination interface, negatively impacting device performance, particularly under anode illumination due to charge transport imbalances. Moreover, electrical measurements have revealed recombination processes occurring within the device structure.
Our investigation is of utmost importance in the quest for achieving comparable performance values in semitransparent solar cells. By understanding the underlying causes of Jsc asymmetry and the formation of donor-rich regions, we can take significant strides towards improving the overall performance of these cells. Such advancements are vital for ensuring the suitability of semitransparent solar cells for a wide range of potential applications, where consistent and balanced performance is essential.

References:

1. Cui, Y. *et al.* Wide-gap non-fullerene acceptor enabling high-performance organic photovoltaic cells for indoor applications. *Nat. Energy* **4**, 768–775 (2019).
2. Bergqvist, J. *et al.* Asymmetric photocurrent extraction in semitransparent laminated flexible organic solar cells. *npj Flex. Electron.* **2**, (2018).
3. Rodríguez-Martínez, X. *et al.* Air Processing of Thick and Semitransparent Laminated Polymer:Non-Fullerene Acceptor Blends Introduces Asymmetric Current–Voltage Characteristics. *Adv. Funct. Mater.* 2301192 (2023) doi:10.1002/ADFM.202301192.

P 2.28

Quantitative Determination of Influenza Virus by a Portable Device Based on EGOFET-Aptasensors

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The demand for new biological and chemical sensors is constantly growing in the world. Despite the variety of biosensors provided by using of different combinations of bioreceptors, transducers, materials, and detection systems there are still many restrictions that hinder further development of the field and limit biosensors in the market. Electrolyte gated organic field effect transistors (EGOFETs) are a promising platform for ultrasensitive, fast and reliable detection of biological molecules by low cost, point-of-care bioelectronic sensors, and can provide an alternative to expensive and complex complementary metal oxide semiconductor-based electronics [1].

EGOFETs biosensitivity is achieved by modification of one of the transistor active interfaces – gate or organic semiconductor surface (OSC). Here we used functionalization of the OSC with bioreceptors to pave the way of creation of compact planar device for lab-on-chip design. The fabrication process of the bioreceptor layer, based on biotin-streptavidin interaction, was developed by us earlier [2, 3].

To meet the demand of recognition properties we have used linker elements like nucleic acid aptamers, that demonstrate high affinity and specificity to the target virus of influenza A. Examples of successful implementation of the aptamers in biosensors (so called aptasensors) can be illustrated for detection of viruses [2, 4]. Aptasensors are able to detect a few viral particles in the sample with a limit of detection of 10-100 viral particles per mL or 2-5 viral particles per mL within 15 minutes [5].

Since the devices biofunctionalization was realized through the OSC layer, the influence of the thickness of an active layer is discussed. The sensitivity and selectivity of the devices were examined with influenza A virus and control bioliquids like NDV virus, virus of influenza B, allantois liquid with different dilutions. The fabrication of a flow cell that registers the response from several devices on the sample simultaneously brings us closer to the creation of a multi-sensor flow device [6]. The preliminary results obtained in the flow mode measurements showed reliable response to virus presence [7].

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References

[1] E. Macchia and L. Torsi, "Biochemical Sensing" (Melville, New York, 2022), Chap. 5.
[2] E.Y. Poimanova et al., "Biorecognition Layer Based On Biotin-Containing [1]Benzothieno[3,2-b][1]benzothiophene Derivative for Biosensing by Electrolyte-Gated Organic Field-Effect Transistors", ACS Appl. Mater. Interfaces, **14**, 16462 (2022).
[3] E.Y. Poimanova et al., "Electrolyte-gated organic field-effect transistors based on 2,6-dioctyltetrathienoacene as a convenient platform for fabrication of liquid biosensors", Russ. Chem. Bull. **71**, 2116 (2022).
[4] B. Lou et al. "Aptamer-based biosensors for virus protein detection", Trends Analyt. Chem. **157**, 116738, (2022)
[5] V. Kukushkin et al. "Multiplex lithographic SERS aptasensor for detection of several respiratory viruses in one pot", Int. J. Mol. Sci. **24**, 8081 (2023).
[6] P.A. Shaposhnik et al. "Applying of C8-BTBT-Based EGOFETs at Different pH Values of the Electrolyte", Chemosensors **11**, 74 (2023).
[7] E.Y. Poimanova et al., "EGOFET-based Aptasensors for Quantitative Determination of Influenza Virus by a Portable Device" Chemosensors, submitted.

P 2.29

Raman Spectroscopy of Electrolyte-gated graphene for protein detection

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Graphene sensitivity to the external environment has been extensively exploited in several sensors' technologies. In our work we propose a novel biological sensor platform for the detection of biomarkers, based on single layer graphene capacitively coupled with a sensing electrode, using Raman spectrum as measured signal. Recent works reported Kelvin probe measurements of the workfunction shift of functionalized metal electrodes following the binding of analyte molecules with recognition elements [1]; it has been proved to be one crucial effect contributing to the transduction of biological events into measurable signals, and its magnitude is now provided. On the other hand, the electric field tuning of graphene Fermi energy is a well-known phenomenon revealing graphene's sensitivity to electrostatic external environment [2-3]. Those knowledge have inspired the design of the proposed device, consisting of a sensing interface and a single layer graphene, capacitively coupled via deionized water working as gating electrolyte. It makes use of the highly sensitive response of the Raman spectrum of graphene to applied electric field to probe electrostatic modifications occurring at the functionalized interface upon binding events. A physical model of the device is presented with a description of its working principle as a biosensor; simulations of the expected results from a sensing experiment have been computed. Preliminary sensing experiments have been performed for the detection of human immunoglobulin M (IgM) and results are presented.

References

[1] *Di Franco C. et al, Extended Work Function Shift of Large-Area Biofunctionalized Surfaces Triggered by a Few Single-Molecule Affinity Binding Events. Adv. Mater. Interfaces, 2023, 10, 2201829, doi:10.1002/admi.202201829*

[2] *Froehlicher G. and Berciaud S., Raman Spectroscopy of Electrochemically Gated Graphene Transistors: Geometrical Capacitance, Electron-Phonon, Electron- Conclusion Electron, and Electron-Defect Scattering. Phys Rev B, 2015, 91, doi:10.1103/PhysRevB.91.205413*

[3] Yan J. et al, Electric Field Effect Tuning of Electron-Phonon Coupling in Graphene. Phys Rev Lett, 2007, 98, doi:10.1103/PhysRevLett.98.166802

Towards a Deeper Understanding of the Ionic Charging in Naphthalenediimide-Based N-Type Conjugated Polymer Electrodes

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Conjugated polymers with hydrophilic side chains are a type of organic mixed ionic/electronic conductors (OMIECs) that is attracting interest for applications in organic electrochemical transistors, electrochromic devices and energy storage devices. Compared with numerous stable and high-performance p-type mixed-conducting polymers, n-type mixed-conducting polymers usually suffer from poor stability in water and air. To date, most reported solution processable n-type mixed conducting polymers that show good stability, high electron mobility and high specific capacity, involve the naphthalenediimide (NDI) unit. [1-3] However, NDI-based mixed-conducting polymers vary in their performance and their mechanical and electrochemical stability with varying molecular designs and electrolyte choice. The underlying mechanisms by which polymer side chains and backbones facilitate ion/electron transport and storage, and by which ionic charging/discharging deteriorates the stability are not fully understood. Thus, to identify the microscopic interactions controlling the overall performance and extract design rules for further material and device optimisation, *operando* characterisation methods and multiscale models are required. In this work, we study several NDI-based n-type mixed conducting polymers with different side chain and backbone structures operating in aqueous electrolytes of systematically varying concentrations to control both the mechanical and electrochemical stabilities. We observe that increasing electrolyte concentration and replacing a small fraction of hydrophilic side chains with hydrophobic ones largely improve the performance and stability of the NDI-based n-type mixed conducting polymers. This improvement can be tentatively attributed to a reduction in swelling, which avoids excessive electrolyte uptake, thereby improving the environment for ion transport and maintaining the intermolecular connections. We propose design rules for both material and electrolyte to maximise reversible multi-electron charging of n-type mixed conducting polymers.

References

[1] D. Moia, "Design and evaluation of conjugated polymers with polar side chains as electrode materials for electrochemical energy storage in aqueous electrolytes", *Energy Environ. Sci.* **12**, 1349-1357 (2019).

[2] I. P. Maria, "The Effect of Alkyl Spacers on the Mixed Ionic-Electronic Conduction Properties of N-Type Polymers", *Adv. Funct. Mater.* **31**, 2008718 (2021).

[3] A. A. Szumska, "Reversible Electrochemical Charging of n-Type Conjugated Polymer Electrodes in Aqueous Electrolytes", J. Am. Chem. Soc. **143**, 14795-14805 (2021).

P 3.2

Electric Field Induced Negative Capacitance in Semiconducting Polymer

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Electric field dependent capacitance and dielectric loss in poly(3-hexylthiophene) are measured by precision capacitance bridge. Carrier mobility and density are estimated from fits to current-voltage and capacitance data. The capacitance varies largely at lower frequency, and it decreases at higher electric fields. The negative capacitance at low frequency and high field is due to the negative phase angle between dipole field and ac signal. The intrinsic carrier density is calculated from fits to the Mott-Schottky equation, and this is consistent with *I-V* data analysis. At higher frequency, the carriers do not follow the ac signal and its density drops; and the flat band potential increases mainly due to the built-in potentials within ordered and amorphous regions in the sample [1].

Reference

[1]. **Sougata Mandal** and Reghu Menon, *Journal of Applied Physics*, **133,** 095102, (2023).

P 3.3

Transport Layer Engineering Towards Lower Threshold for Perovskite Lasers

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Metal halide perovskites have emerged as a promising candidate for future lasers owing to various advantages such as low-cost solution processability, bandgap-tunable luminescence with high color purity and high photoluminescence quantum yields (PLQY), outstanding optical gain coefficient, and excellent optoelectronic properties.[1] With intensive research interests, two significant breakthroughs have been made: the achievement of room temperature optically pumped continuous-wave lasers[2], and the realization of high injection current densities (>1 kA/cm^2)[3]. These breakthroughs make halide perovskites very promising for electrically pumped lasers. Towards demonstrating electrically pumped lasers, it is necessary to sandwich the perovskite thin film into transport layers for the integration of electrical devices. However, it remains unclear how transport layers will influence perovskite lasing actions.

In this talk, I will present the role of charge transport layers on the lasing actions of perovskite films by investigating the amplified spontaneous emission (ASE) thresholds. We demonstrate a largely reduced ASE threshold and enhanced ASE intensity by introducing an additional hole transport layer poly(triaryl amine) (PTAA). We show that the key role of the PTAA layer is to accelerate the hot carrier cooling process by extracting holes in perovskites. With reduced hot holes, the Auger recombination loss is largely suppressed, resulting in decreased ASE threshold. Our argument is further supported by the fact that the ASE threshold can be further reduced from 25.7 to 7.2 μJ/cm^2 upon switching the pumping wavelength from 400 nm to 500 nm to directly avoid excess hot hole generation. Our work[4] for the first time exemplifies how to further reduce the ASE threshold with transport layer engineering through hot hole manipulation. This is critical to maintaining the excellent gain properties of perovskites when integrating them into electrical devices, paving the way for electrically pumped perovskite lasers.

References

[1] W. B. Gunnarsson, B. P. Rand, “Electrically driven lasing in metal halide perovskites: Challenges and outlook,” *APL Mater.* **8**, 030902 (2020).

[2] C. Qin, A. S. D. Sandanayaka, C. Zhao, T. Matsushima, D. Zhang, T. Fujihara, C. Adachi, “Stable room-temperature continuous-wave lasing in quasi-2D perovskite films,” *Nature* **585**, 53 (2020).

[3] L. Zhao, K. Roh, S. Kacmoli, K. Al Kurdi, S. Jhulki, S. Barlow, S. R. Marder, C. Gmachl, B. P. Rand, “Thermal management enables bright and stable perovskite light-emitting diodes,” *Adv. Mater.* **32**, 2000752 (2020).

[4] J. Zhang, J. Qin, W. Cai, Y. Tang, H. Zhang, T. Wang, A. Bakulin, B. Hu, X.-K. Liu, F. Gao, “Transport layer engineering towards lower threshold for perovskite lasers,” *Adv. Mater.* DOI: 10.1002/adma.202300922 (2023).

P 3.4

Fill factor limit in organic solar cells

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Organic solar cells (OSCs) have enabled a high power conversion efficiency (PCE) of around 20%[1]. The ever-increasing efficiency has been accompanied by a deeper understanding of the dominant performance parameters, including the open-circuit voltage (V_{OC}), short-circuit current (J_{SC}) and fill factor (FF). However, the relationship between these parameters is complex and often involves trade-offs. In particular, the FF in OSCs appears to compete with the V_{OC}, which differs from other semiconductors [2,3].
For an efficient solar cell, the requirements of V_{OC} and FF are consistent in terms of reducing recombination losses. Previous analytical expressions have shown that a higher FF is achievable with a higher V_{OC}. Indeed, for solution-processed perovskite solar cells, suppressed V_{OC} losses are associated with increased FF[4]. It seems conceivable that reducing the V_{OC} loss is always beneficial to the maximum FF available in a solar cell. However, this does not apply to OSCs. Reports show that increasing V_{OC} can be detrimental to FF in OSCs, contradicting what has been observed in inorganic and hybrid semiconductors. This raises two important questions: i) what causes this limit and ii) how it can be avoided.

In this work, we explore the FF limit in OSCs. We analyze a large quantity of OSCs with voltage loss from 0.5 eV to 1.1 eV and FF from 0.27 to 0.8. We find that transport limit cannot explain the unique FF limit in organics. We select four representative systems based on Y6-series NFAs with low V_{OC} loss. We investigate the charge generation process in these systems and observe an emissive bound state that is suggested to be a hybrid state of local excited (LE) and charge transfer (CT) states. This weakly bound state shows field-dependent charge generation, which is a unique feature in OSCs that causes FF loss besides transport-limit. Moreover, the weakly bound state can influence the transport-limit by reseparating into free charge carriers. The reseparation would reduce recombination coefficient, and its reduction degree is proportional to the dissociation probability of the bound state.

References

[1] Wang, J., Wang, Y., Bi, P., Chen, Z., Qiao, J., Li, J., Wang, W., Zheng, Z., Zhang, S., Hao, X. and Hou, J., "Binary Organic Solar Cells with 19.2% Efficiency Enabled by Solid Additive," Advanced Materials **2301583** (2023).
[2] Eisner, F.D., Azzouzi, M., Fei, Z., Hou, X., Anthopoulos, T.D., Dennis, T.J.S., Heeney, M. and Nelson, J., "Hybridization of local exciton and charge-transfer states reduces nonradiative voltage losses in organic solar cells," Journal of the American Chemical Society, **141**, 6362-6374 (2019).
[3] Classen, A., Chochos, C.L., Lüer, L., Gregoriou, V.G., Wortmann, J., Osvet, A., Forberich, K., McCulloch, I., Heumüller, T. and Brabec, C.J., "The role of exciton lifetime for charge generation in organic solar cells at negligible energy-level offsets," Nature energy, **5**, 711-719 (2020).
[4] Green, M.A., "Accuracy of analytical expressions for solar cell fill factors. Solar cells," **7**, 337-340 (1982).

P 3.5

Title in Arial, Bold, 16-Point Type and Centered, Upper and lower cases

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Two-dimensional metal halide perovskites (2DHPs) are a class of crystalline materials that consist of metal halide octahedral layers that are separated by bulky organic cations to stabilise the structure and control the interlayer spacing. Similar to three-dimensional (3D) perovskites, the ability to tune the bandgaps by controlling the halide composition can also be applied in 2DHPs, which further broad their potentials in real applications. The spatially separated octahedral layers in 2DMHPs confine the exciton-lattice interactions along the in-plane octahedral direction, which further confine the halide migration pathway within in-plane. In this work, we quantitively identify the crystallisation of mixed halide 2DHPs following a unique strategy with bromine preferentially taking the equatorial position while iodine taking the axial position. We report halide positions within the octahedral can be actively tuned between axial and equatorial positions with light through the strong exciton-lattice interactions in 2DHPs, and we investigate the lattice modulation depth by in situ monitoring the change of emission bandwidth and halide positions within the structure. Our work creates a new pathway for the application of 2DHPs in lithography-free photonics, optical switching, LED and memory applications.

P 3.6

Solvatochromic Emission from the "Dark" Double-Exciton State of a Polyhalogenated Thiele Hydrocarbon: a joint Quantum-Chemical and Experimental Investigation

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Recently there has been a considerable interest in the exploration of organic neutral radicals for various applications including optoelectronics [1]. Radical-based OLEDs can reach values of internal quantum efficiency of 100% [2], but two major unsolved problems affect these devices: a severe roll-off and a device lifetime of few minutes [1,3]. An alternative to free radicals, potentially capable to overcome these problems, is represented by luminescent diradicaloids. Here we present a computational investigation on the luminescence properties of the first example of an inert and photostable non-perchlorinated Thiele hydrocarbon (TTH) recently synthesized [4]. This molecule exhibits an intense solvatochromic emission with a large Stokes shift of ca. 0.66 eV. Diradicals have attracted considerable attention due to their potential applications in optoelectronic devices [5] and in singlet fission process [6]. The luminescence properties of TTH have been interpreted with quantum-chemical (QC) calculations demonstrating the key role of its moderate diradical character in determining the unconventional fluorescence properties. QC calculations suggest that a mixing of the bright state responsible for the absorption spectrum with a low-lying double-exciton state (dominated by H,H→L,L configuration) [7], assisted by the twisting around one of the two (strongly elongated) exocyclic CC bonds of TTH, drives the formation of the emitting species which (because of state mixing) acquires a charge-separated character, accounting for the observed solvatochromism. Such charge separation occurs therefore with a mechanism similar to sudden polarization [8]. Interestingly, *fs* and *ns* transient absorption spectroscopy unambiguously show the involvement of two excited states and strongly support the twisting-induced mixing in the deactivation pathways of TTH, in excellent agreement with computational results. We believe that understanding the luminescence mechanism in TTH will contribute to design *p*QDM derivatives and related conjugated diradicaloids with increased luminescence efficiency.

References

[1] J. M. Hudson, et al. J. Appl. Phys. **129,** 180901 (2021)
[2] H. Guo, et al., Nat. Mater. **18**, 977 (2019)
[3] X. Ai, et al., Nature **563**, 536
[4] A. Punzi, Y. Dai, C. N. Dibenedetto, E. Mesto, E. Schingaro, M. Striccioli, T. Ullrich, D. M. Guldi, F. Negri, G. M. Farinola, D. Blasi, *Submitted*
[5] (a) Y. Huang, et al., Polym. J. **50,** 603 (2018); (b) X. Hu, et al., J. Mater. Chem. C **6,** 11232 (2018)
[6] S. Lukman, et al., J. Am. Chem. Soc. **139**, 18376 (2017)
[7] (a) F. Negri, et al., in *Diradicaloids* (ed. J. Wu, Jenny Stanford Publishing 2022), Chap. 3; (b) S. Canola et al., Phys. Chem. Chem. Phys. **20**, 24227 (2018)
[8] M. Filatov, et al., J. Chem. Theory Comput. **17**, 5123 (2021)

P 3.7

Influence of ligand exposure on the mechanical properties of biofunctionalized interfaces

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Biofunctionalized interfaces play a pivotal role in the development of sensing devices, enabling accurate detection and quantification of various biological biomarkers even at the physical limit of single molecule detection. [1] A fundamental aspect in the design and optimization of these interfaces is the comprehension of the mechanical properties exhibited by physiosorbed protein layers. Indeed, understanding the mechanical behavior of these biofilms is crucial since it directly impacts their stability, performance, and overall functionality.

In this study, we aim to investigate the effects of ligand exposure on the mechanical properties of gold surfaces functionalized with anti-IgG antibodies. The IgG antigens, which specifically bind to the immobilized antibodies, can significantly influence the structure and mechanical properties of the biofilm. By exposing the biolayer to the ligands, we can explore the alterations in the distribution of Young modulus and adhesion forces and gain insights into the dynamic response of the biofunctionalized interface.

Experimental analysis will involve the fabrication of biofunctionalized interfaces with controlled protein layers and subsequent exposure to specific ligands. Atomic Force Microscopy (AFM) and Force Spectroscopy (FS) will be employed to achieve the quantitative nanomechanical mapping of protein layer to estimate its mechanical properties, including Young's modulus and adhesion. The outcomes of this study will contribute to advancing our understanding of the mechanical behavior of biofunctionalized interfaces and provide valuable insights into the effects of ligand exposure on their stability and performance. These results can support the development of more robust and efficient sensing devices, with potential applications biomedicine, environmental monitoring, and diagnostics.

References

[1] Macchia, E. et al. Large-Area Interfaces for Single-Molecule Label-free Bioelectronic Detection. Chem. Rev. (2022) doi:10.1021/acs.chemrev.1c00290

P 3.8

Substrate Transfer of Graphene Nanoribbons (GNRs): A Key Step in the Integration-to-devices Process

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Graphene nanoribbons (GNRs) have received special attention as promising materials for opto-electronics applications, since a smart control of their width and edge structure enables a fine tune of their properties. Bottom-up approaches based on on-surface synthesis have allowed to prepare a wide variety of GNRs with atomic precision, while the coupling to scanning probe techniques have permitted to study their properties at the single-molecule level. Nevertheless, examples of their successfully implementation to real devices are still scarce in literature. In this sense, the GNR transfer to different surfaces other than those on which they were grown is one of the most challenging steps. The success of this transfer mainly depends on the conservation of the GNR quality, as well as achieving a high transfer efficiency, while preserving the alignment and orientation of the GNRs. All these factors have a direct impact in the final-device performance.

In this work, we present different strategies towards the effective and reliable transfer of GNRs,[1] [2] which have been successfully applied by our group for their integration to devices,[3] highlighting the key role of Raman spectroscopy as powerful tool for following the quality of the GNRs along the process.

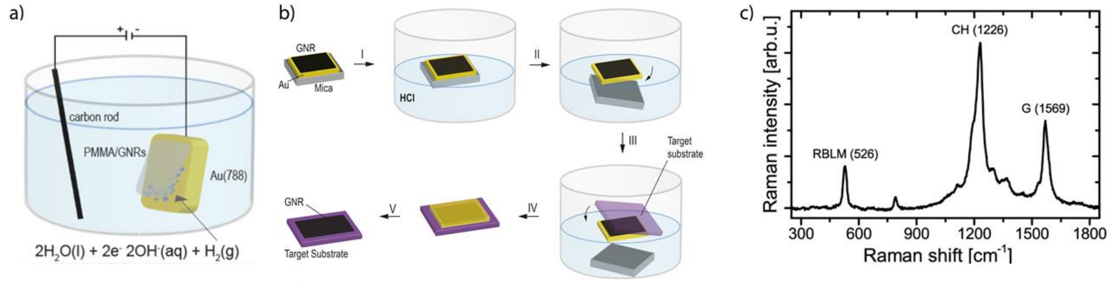

Figure 1: Schematic representation of a) an electrochemical delamination method to GNR transfer from gold to PMMA and b) a polymer-free GNR transfer protocol. c) Raman spectra of transferred GNRs.

References

[1] Borin Barin, Gabriela; Fairbrother, Andrew; Rotach, Lukas; Bayle, Maxime; Paillet, Matthieu; Liang, Liangbo; Meunier, Vincent; Hauert, Roland; Dumslaff, Tim; Narita, Akimitsu; Müllen, Klaus; Sahabudeen, Hafeesudeen; Berger, Reinhard; Feng, Xinliang; Fasel, Roman; Ruffieux, Pascal; *ACS Appl. Nano Mater*. **2019**, 2, 4, 2184–2192.

[2] El Abbassi, Maria; Perrin, Mickael L.; Borin Barin, Gabriela; Sangtarash, Sara: Overbeck, Jan; Braun, Oliver; Lambert, Colin J.; Sun, Qiang; Prechtl, Thorsten; Narita, Akimitsu; Müllen, Klaus; Ruffieux, Pascal; Sadeghi, Hatef; Fasel, Roman; Calame, Michel; *ACS Nano* **2020** 14 (5), 5754-5762

[3] Borin Barin, Gabriela, Sun, Qiang., Di, Marco., Cheng-Zhuo Du, Wang, Xiao-Ye; Llinas, Juan P.; Mutlu, Zafer; Lin, Yuxuan; Wilhelm, Jan; Overbeck, Jan; Daniels, Colin; Lamparski, Michael; Sahabudeen, Hafeesudeen; Perrin, Mickael L.; Urgel, José I.; Mishra, Shantanu; Kinikar, Amogh; Widmer, Roland; Stolz, Samuel; Bommert, Max; Pignedoli, Carlo; Feng, Xinliang; Calame, Michel; Müllen, Klaus; Narita, Akimitsu; Meunier, Vincent; Bokor, Jeffrey; Fasel, R., Ruffieux P.; *Small* **2022**, 18, 2202301.

P 3.9

Donor-Acceptor-Donor Triads with Flexible Spacers: Deciphering Complex Photophysics for Targeted Materials Design

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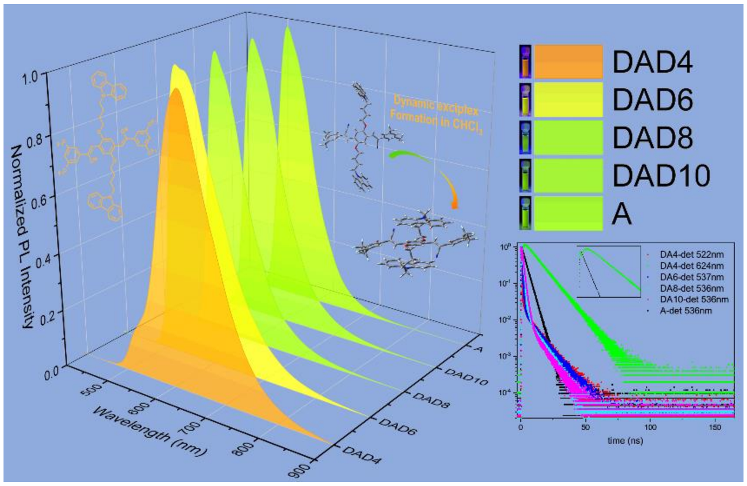
Over the past years, dual emission (DE) of organic conjugated molecules has attracted much attention for use in optoelectronics. In the current work, we report DE by two correlated emitters in donor-acceptor-donor (D-A-D) molecular triads, based on carbazole (D), and cyano-distyrylbenzene (A). UV/Vis absorption and quantitative steady-state and time-resolved fluorescence spectroscopy, combined with time-dependent density functional theory (TD)DFT calculations are used to elucidate the intriguing DE phenomenon; competing photoinduced electron transfer and charge transfer (CT) formation lead to DE from the locally excited (LE) state and the exciplex, revealing a significant dependence on varying D-A linker length and temperature.[1-2]



References

[1] S. K. Behera, S. Y. Park, J. Gierschner, “Dual Emission: Classes, Mechanisms, and Conditions,” Angew. Chem. Int. Ed **60,** 22624 (2021).

[2] M. S. Kwon, J. Gierschner, S.-J. Yoon, S. Y. Park, “Unique Piezochromic Fluorescence Behavior of Dicyanodistyrylbenzene Based Donor–Acceptor–Donor Triad: Mechanically Controlled Photo-Induced Electron Transfer (eT) in Molecular Assemblies,” Adv. Mater **24,** 5487 (2012).

P 3.10

Simplified Fluorene-Based Hole Transport Materials for the Long-Term Stability of Perovskite Solar Cells

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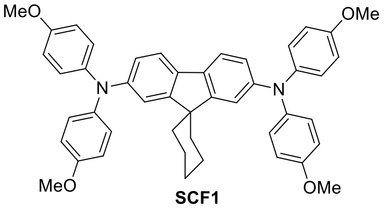
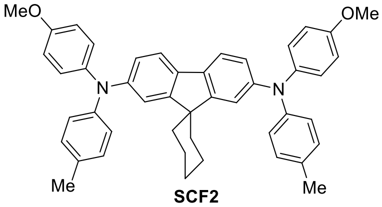
Halide perovskite solar cells (PSCs) have made significant advancements, achieving a certified power conversion efficiency (PCE) of 25.7%, placing them *on par* with the long-standing silicon photovoltaics. Despite the notable advancements in the performance and fabrication of PSCs, their limited stability remains a major obstacle to their widespread use. The interfaces between the perovskite layer and the adjacent charge transport materials have proved crucial in governing the durability and longevity of these devices.[1] A huge research effort has been devoted to the design of Hole Transporting Materials (HTM) for PSCs, aiming at overcoming the drawbacks connected to the use of Spiro-OMeTAD or PTAA-based materials, which to date represent the most common HTM but are expensive, require complex synthesis under harsh conditions, and rely on hygroscopic dopants (such as LiTFSI or tBP) to optimize their hole mobility. In the awareness that a pathway to enhance the efficiency and stability of perovskite solar cells is through the rational design of HTMs that can effectively interact to the perovskite surface, in this communication we will discuss the synthesis, characterization and application of two new molecular architectures (**SCF1** and **SCF2**) based on the fluorene *motif*, and inspired from the aforementioned Spiro-OMeTAD structure, aiming to create compact and well-ordered interfaces in PSCs.



SCF1



SCF2

The synthesis of our novel HTMs was achieved using a convergent approach that involved sequential Buchwald-Hartwig aminations and the cost analysis revealed that **SCF1** and **SCF2** were obtained at 29 €/g and 33 €/g, respectively, considerably lower compared to the estimated cost of Spiro-OMeTAD. When SCF-HTMs were employed as thin layers in n-i-p structure PSCs with the triple-cation halide perovskite CsFAMA, in dopant-free conditions, the champion **SCF1**-based unencapsulated devices displayed an impressive shelf-stability with a T_{80} lifetime of 431 days, while the performance of doped Spiro-OMeTAD-based devices, on the other hand, degraded over time.[2] This result that could be associated to the stable interface formed with the CsFAMA surface, as also supported by theoretical insights of the interactions between our SCF-HTMs and the modeled perovskite, compared to those involving the reference Spiro-OMeTAD.

References

[1] S. Shao, M. A. Loi, *The Role of the Interfaces in Perovskite Solar Cells*, Adv. Mater. Interfaces **7**, 1901469 (2020).
[2] P. Mäkinen et al., *Less Is More: Simplified Fluorene-Based Dopant-Free Hole Transport Materials Promote the Long-Term Ambient Stability of Perovskite Solar Cells*, Chem. Mater. **35**, 7, 2975–2987 (2023).

P 3.11

Mechano-reaction at a single molecular level: Forcing a Molecule to isomerize under application of external mechanical force.

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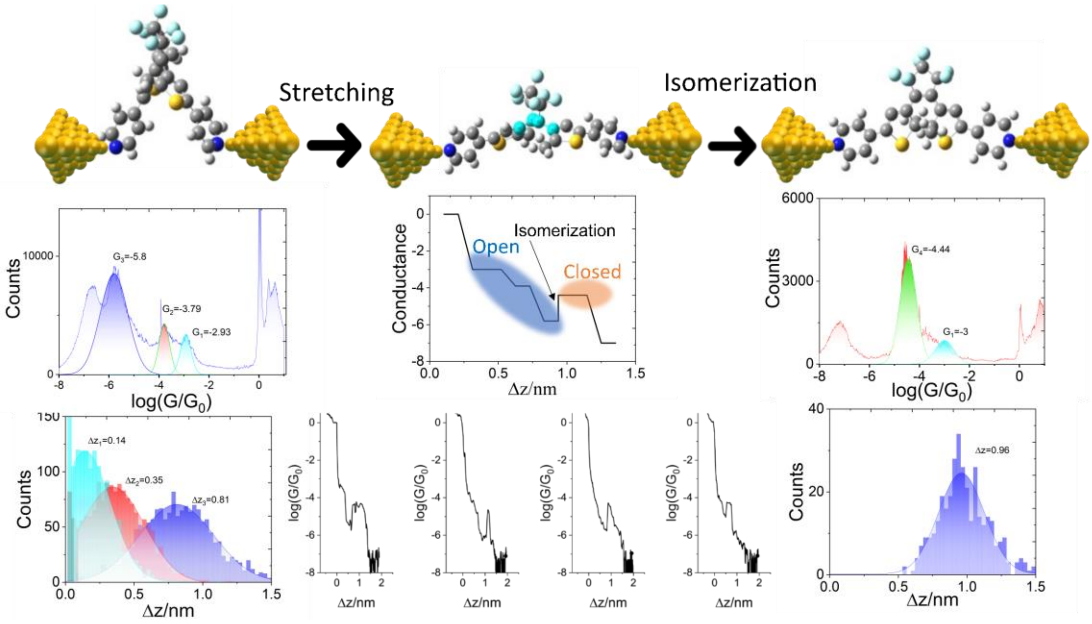
Mechanical force has been long used by various experimentalists to initiate various chemical reactions.Mechanically induced reactions have attracted increased attention due to their solution free, low-temperature, environmental friendly,energy saving andhigh-productionoutput nature.[1] These reactions are quite prevalent in solid state reactions and polymer mechanochemistry. However, in both of these approaches the force applied is not specific and is applied to the bulk to perform the reaction. As a result, there is limiting understanding of the mechanochemical process in these approaches[1,2]. In break junction techniques as the single molecule is trapped between atomically sharp electrodes[3] and these electrodes can be used to impart miniature of force to the very reaction centre of the trapped molecular system. This way the mechanical force can be used to initiate a reaction at a single molecular level and the process can be studied simultaneous by measuring the charge transport during the application of the force.



Using mechanically controlled beak junction technique we have showed that in case of a Dithienylethene derivative molecular system the open form can be forced to undergo 6π electrocyclization to closed form. The flexible open form can be stretching by attaching it to the Au electrodes via pyridine anchoring groups. Upon increasing the electrode-electrode separation the shorter open form is stretching and undergoes isomerisation to longer closed form to relieve the transient molecular strain. The isomerisation events under application of external mechanical force are captured in the single molecular conductance measurements.

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(1) Mateti, S.; Mathesh, M.; Liu, Z.; Tao, T.; Ramireddy, T.; Glushenkov, A. M.; Yang, W.; Chen, Y. I. Mechanochemistry: A Force in Disguise and Conditional Effects towards Chemical Reactions. *Chem. Commun.***2021**, *57* (9), 1080–1092.

(2) O'Neill, R. T.; Boulatov, R. The Many Flavours of Mechanochemistry and Its Plausible Conceptual Underpinnings. *Nat. Rev. Chem.***2021**, *5* (3), 148–167.

(3) Rashid, U.; Chatir, E.; Medrano Sandonas, L.; Sreelakshmi, P.; Dianat, A.; Gutierrez, R.; Cuniberti, G.; Cobo, S.; Kaliginedi, V. Dithienylethene-Based Single Molecular Photothermal Linear Actuator. *Angew. Chem. Int. Ed.***2023**, *62* (16), e202218767.

P 3.12

Quinoxaline-based compounds for TADF emitters

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In recent years, organic light emitting diodes (OLEDs) have attracted increasing interest as the promising devices for full-color display and solid-state lighting technologies. A major breakthrough in OLED technology occurred with the development of OLEDs based on thermally activated delayed fluorescence (TADF) by Adachi and co-workers [1]. Therefore, attention has been drawn to the design and synthesis of various emissive donor–acceptor (D - A) type organic compounds.
TADF becomes highly complicated in solid-state, and these issues still are very scarcely studied. Regardless of the selected D and A units and their linking patterns, the pronounced conformational disorder occurs in solid films [2] which causes temporal shifts of the emission peak and, therefore, results in unwanted effects, such as broadening of the emission spectrum and the prolongation of TADF lifetime [3]. All this makes the control of conformational disorder highly important for the successful application of TADF compounds, especially as emitters in OLEDs. Accordingly, investigation of the properties of the solid and liquid solutions of TADF compounds is of great importance.

Dibenzo[a,c]phenazine and quinoxaline units were chosen as acceptor core because of high rigidity and coplanar π-conjugated structure, which favors the reduction of the band gap and emission in red region. [4]

In this work, aiming to develop efficient materials for TADF emitters, we present donor-acceptor type quinoxaline-based derivatives. The structures were designed, synthesized and characterized by the different theoretical and experimental techniques. Effect on TADF phenomenon by chemical and environmental (solid or liquid) changes of the molecule was determined.

Acknowlegment:

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References

[1] Uoyama, H., Goushi, K., Shizu, K., Nomura, H.; Adachi, C, “Highly efficient organic light-emitting diodes from delayed fluorescence”, Nature **492**, 234-238 (2012).
[2] Serevicius T., Skaisgiris R., Dodonova J., Jagintavičius L., Bucevicius J., Kazlauskas K., Jursenas S., Tumkevicius S., “Emission wavelength dependence on the rISC rate in TADF compounds with large conformational disorder”, Chemical Communications **55**,1975-1978 (2019).
[3] Serevicius T., Buciunas T., Bucevicius J., Dodonova J., Tumkevicius S., Kazlauskas K., Jursenas S., “Room temperature phosphorescence vs. thermally activated delayed fluorescence in carbazole–pyrimidine cored compounds”, Journal of Materials Chemistry C **6**,11128–11136 (2018).
[4] Xie, F.M., Li, H.Z., Dai, G.L., Li, Y.Q., Cheng, T., Xie, M., Tang, J.X., Zhao, X. “Rational molecular design of dibenzo[a,c]phenazine-based thermally activated delayed fluorescence emitters for orange-red OLEDs with EQE up to 22.0%”, ACS Applied Materials & Interfaces **12 (16),** 18730–18738 (2020).

P 3.13

Molecular topology for the construction of organic semiconductor: design and synthesis

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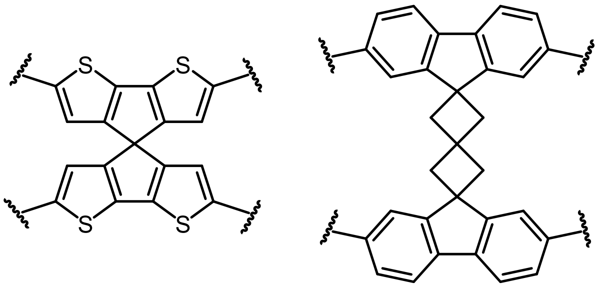
Organic semiconductor based photovoltaic technology has been considered as the next generation renewable energy technology for the advantages of low cost, light weight, and easy of large area fabrication[1]. Most of the organic semiconductors used in organic photovoltaic (OPV) are 1D linear conjugated polymer or small molecules. Increasing the molecular dimensionality of the organic semiconductor molecules is expected to increase the light harvesting ability, the charge carrier mobility of the materials, and long-term stability, which would be beneficial for OPV performance[2,3]. This poster presents the design and synthesis of some 3-dimensional (3D) building blocks and their application in the preparation of organic semiconductor materials. The core structures include the 3D 4,4'-spirobi[cyclopenta[2,1-*b*:3,4-*b*']dithiophene] (**SCT**), and 3D trispiro[fluorene-9,1'-cyclobutane-3',1''-cyclobutane-3'',9'''-fluorene] (**SDF**). Based on them, a series of A-π-D-π-A structure organic semiconductor molecules were synthesized. Through the study of the photophysical and electrochemical properties of this series of derivatives, the molecular orbital energy level and energy level bandwidth of the compound were determined and the results show that these materials have the potential to be applied in optoelectronic devices.



SCT **SDF**

Figure 1. Example structures of the core building block

References

[1] Liu, C.; Xiao, C.; Xie, C.; Li, W., Flexible organic solar cells: Materials, large-area fabrication techniques and potential applications. *Nano Energy* **2021**, 89, 106399..

[2] Chen, H.; Zhang, Z.; Wang, P.; Zhang, Y.; Ma, K.; Lin, Y.; Duan, T.; He, T.; Ma, Z.; Long, G.; Li, C.; Kan, B.; Yao, Z.; Wan, X.; Chen, Y., 3D acceptors with multiple A–D–A architectures for highly efficient organic solar cells. *Energy Environ. Sci.* **2023**, 16 (4), 1773-1782.

[3] Qi, F.; Li, Y.; Zhang, R.; Lin, F. R.; Liu, K.; Fan, Q.; Jen, A. K.-Y., Dimer Acceptor Adopting a Flexible Linker for Efficient and Durable Organic Solar Cells. *Angew. Chem., Int. Ed.* **2023**, 62 (21), e202303066.

P 3.14

High charge carrier mobility of multilayered random network of MXene flakes casted from water solution

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Solution processable two-dimensional materials have great potential in the application of printed electronic elements. Typically their electrical properties like e.g. charge mobility of this randomly oriented network of flakes is significantly lower than in a single flake of the same material. Nevertheless we have prepared layers comprising multi-layered, randomly oriented Ti_3C_2 MXene flakes and characterized charge carrier transport in them[1]. The results of time-of-flight photoconductivity measurements confirm electron transport with mobilities up to 279 cm^2/Vs, which is substantially higher than previously reported field-effect mobility, which was below 10 cm^2/Vs. Mobility was increasing with electric field - characteristic to disordered materials. The extrapolated zero-field mobility of 38 ± 15 cm^2/Vs reaches values measured in single $Ti_3C_2T_x$ MXene flakes (34 cm^2/Vs). We suggest that this is a consequence of precise MXene exfoliation and efficient deposition process. The exfoliation yielded flakes with the largest dimensions on the order of several microns. The deposition of the layers resulted in up to 6-layer-thick film of interconnected randomly oriented flakes. We demonstrate that the transport through such randomly connected percolation network can be characterized as charge transport through crystalline flakes, perturbed by trapping in the localized states, residing at the interfaces between the flakes. The former process results in high charge mobility, the latter results in a low charge carrier mobility. This duality is likely to be responsible for relatively high values of TOFP-measured charge carrier mobility. These results also suggest that charge trapping at the dielectric interface becomes less important when the charge carriers are transported through several pristine MXene layers above and away from the dielectric interface as in our TOFP experiments. This results in overall higher observed charge carrier mobility. On the other side, the charge carrier mobility exhibits positive dependence on the electric field of the Poole-Frenkel type, which is typical for disordered material. This behavior seems to be pertinent to a multilayered network of randomly distributed flakes with an interfacial electronic structure, which does not suppress the charge transport, but it represents a bypass to improved charge carrier transport.

References

[1] J. Urbančič et al., "Time-of-Flight Photoconductivity Investigation of High Charge Carrier Mobility in $Ti_3C_2T_x$ MXenes Thin-Film," Diamond and Related Materials **135**, 109879 (2023).

P 3.15

Quantum Interference Effect in Single Molecule Junctions Containing Multiple Aliphatic Bridges.

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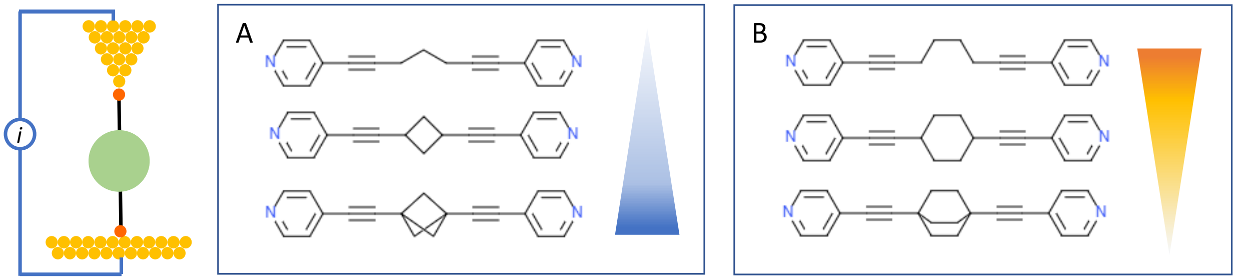
Charge transport through individual molecules or their assemblies represents an important field of nanoscience. At the single molecule level molecular circuits obey quantum physics rather than statistical physics laws. As a consequence, quantum interference (QI) became an important concept in the single molecule electronics. Two sets of molecules with single, double and triple connectors in parallel in the central part of the molecular structure have been studied by Scanning Tunneling Microscopy Break Junction method (STMBJ) and density functional theory combined with the non-equilibrium Green's function formalism in order to understand charge transport properties and provide most probable metal-molecule-metal junction geometries. Each set contains different number of carbon atoms in the conducting bridge. The first set contains -CH_2- and the second set -CH_2-CH_2- unit(s) in the bridge connected to a common carbon on both sides of the bridge as shown in Figure below, see panel A and B.



Multiple conductance pathways in the conventional electrical circuit obey Kirchhoff's law, i.e. the current at the output of parallel branches is the sum of the currents through individual branches. In the case of nanoscale objects the conductance depends on molecular structure and quantum interference (QI) may be observed, where the current has either higher (constructive) or lower value (destructive) compared to that expected by Kirchhoff's law [1–4]. In this work we have observed that single molecule conductance of molecules with increasing number of parallel -CH_2- branches increases, whereas the single molecule conductance of molecules with increasing number of parallel -CH_2-CH_2- branches decreases. This behavior is reminiscent of an odd-even effect observed in organic alkane-based self-assembled monolayers. Quantum chemical calculations were able to reproduce the experimental results and provided an understanding of the essential features of the electron transport in these systems.

Financial support by the Czech Science Foundation (21-13458S) is gratefully acknowledged.

References

[1] H. Vazquez, R. Skouta, S. Schneebeli, M. Kamenetska, R. Breslow, L. Venkataraman, M. S. Hybertsen, "Probing the conductance superposition law in single-molecule circuits with parallel paths," *Nat. Nanotechnol.* **7**, 663-667 (2012).
[2] C. J. Lambert, "Basic concepts of quantum interference and electron transport in single-molecule electronics," *Chem. Soc. Rev.* **44**, 875-888 (2015).
[3] J. Šebera, M. Lindner, J. Gasior, G. Meszáros, O. Fuhr, M. Mayor, M. Valášek, V. Kolivoška, M. Hromadová, "Tuning the contact conductance of anchoring groups in single molecule junctions by molecular design," *Nanoscale* **11**, 12959-12964 (2019).

P 3.16

Outstanding Fill Factor in Inverted Organic Solar Cells with SnO_2 by Atomic Layer Deposition

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The inverted (n-i-p) structure is considered more suitable for the industrial production of organic solar cells (OSCs), due to the superior stability of the materials used in this configuration. Zinc oxide (ZnO) is commonly used as electron transport layer (ETL) in OSCs with this structure, since it can be easily deposited from solution and it is able to provide good device performance. However, when in contact with the active layer, ZnO is known to cause photocatalytic degradation of the organic materials, with a severe effect on the device stability [1]. Tin oxide (SnO_2) can represent a valid alternative to ZnO as ETL, not inducing problems of degradation and offering superior transparency to the visible light and higher electron mobility.

To hinder a broad use of SnO_2 as ETL in OSCs is the difficulty to fabricate films of the material with high crystalline quality. The fabrication of SnO_2 films from solution, with nanoparticle colloidal dispersions, gives rise to films with a high defect density, especially on the surface. Moreover, organic ligands, used to stabilize the nanoparticle dispersions, often leave residuals in the deposited film, which can compromise the interface with the active layer. As a result, the overall performance of OSCs with SnO_2 as ETL is often inferior to that of devices with ZnO, due to substantially lower values of fill factor (FF).

An alternative method to fabricate SnO_2 films, with the desired crystalline quality, is the use of atomic layer deposition (ALD). ALD is an industrial grade technique which can be applied at the wafer level and also in a roll-to-roll configuration. SnO_2 deposited by ALD is attracting attention in the research field of photovoltaic and it is currently used in perovskite [2] and tandem solar cells [3]. Nonetheless, its use in OSCs is scarcely reported and its potential in these devices still need to be evaluated.

In this work, we fabricated highly efficient inverted OSCs with SnO_2 deposited by ALD as ETL. The fabricated devices outperform solar cells with either SnO_2 or ZnO deposited from solution, reaching a best efficiency of 17.26% and a record fill factor of 79%. Furthermore, the OSCs with ALD-SnO_2 show a higher stability under illumination in comparison with those utilizing ZnO. To explain such remarkable results, we carried out an accurate characterization of SnO_2 films and OSCs. Our findings attribute the improved performance and stability to a superior quality of the interface between the ALD-SnO_2 film and the active layer and, thus, to a reduced charge carrier recombination [4].

References

[1] Y. Jiang, et al., "Photocatalytic effect of ZnO on the stability of nonfullerene acceptors and its mitigation by SnO2 for nonfullerene organic solar cells", Mater. Horiz. **6**, 1438-1443 (2019)

[2] J. P. Correa Baena, et al. "Highly efficient planar perovskite solar cells through band alignment engineering", Energy Environ. Sci. **8**, 2928-2934 (2015)

[3] L. Mao, "Fully Textured, Production-Line Compatible Monolithic Perovskite/Silicon Tandem Solar Cells Approaching 29% Efficiency", Adv. Mater. **34**, 2206193 (2022)

[4] L.Di Mario, et al., "Outstanding Fill Factor in Inverted Organic Solar Cells with SnO_2 by Atomic Layer Deposition", Adv. Mater. 2301404 (2023)

P 3.17

Enhancing Response Time in Organic Electrochemical Transistors via Top-Gate Configuration with Printed Solid-State Electrolyte

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Organic electrochemical transistors (OECTs) have garnered considerable attention due to their compatibility with low-cost, printing technology, mechanical flexibility and bio-compatibility for diverse fields of applications, including bioelectronics, biosensing, and neuromorphic computing. However, the reliance on liquid electrolytes in most OECT research hinders their adaptation into integrated circuits, and the use of solid-state electrolytes is considered to result in slower device operation. To address these limitations, we present a novel approach utilizing a top-gate architecture in OECTs with a printed solid-state electrolyte. This approach enables a response time below 100 μs without device scaling or costly patterning processes, e.g., photolithography. Furthermore, we demonstrate that the top-gate configuration can be utilized to independently optimize power consumption, transconductance, and device response time. Our findings shed light on the critical factors influencing OECT speed in both side- and top-gate structures, offering insights into the geometry dependency of OECTs. We anticipate that this work will contribute to advancing OECTs for applications such as high-speed biological signal capture and signal processing using spiking neural networks.

P 3.18

Sustainable Carbon Dots with tunable optical properties as promising materials for agritech and green organic electronics

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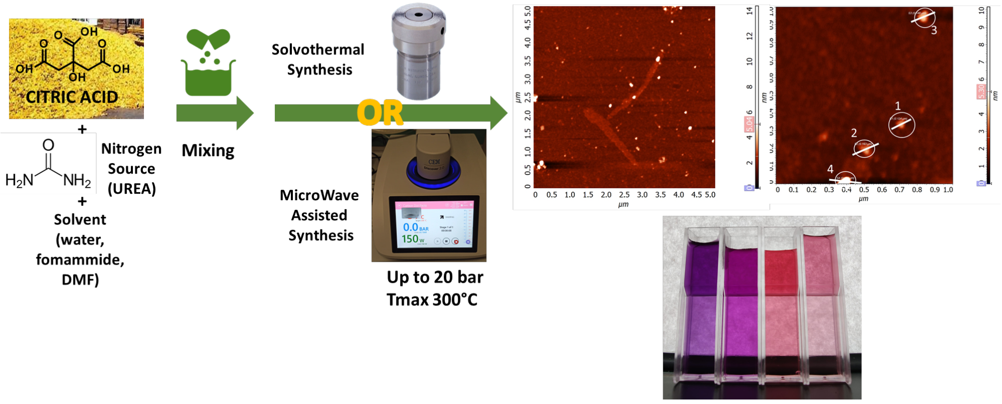

Figure 1. Schematic synthesis of CDs, AFM characterizations water solution of different CDs.

Carbon dots (CDs) are unique nanomaterials with sp2 carbon cores[1] and functional groups, such as amino, hydroxyl and carboxyl on their surface; thanks to their small size (nm) and large surface area they're highly sensitive to the surrounding environment.

CDs exhibit tunable photoluminescence, low toxicity, and biocompatibility, making them valuable in biomedicine[2], catalysis[3], and optoelectronics[4]. Among various application, recent works demonstrate that CDs could affect positively plants growth enhancing germination of seeds through multiple actions: enhancing roots development and nutrient absorption from the soil[5], impacting on photosynthesis generating photocurrent[6].

CDs can be sustainably produced from agricultural waste using microbial fermentation to obtain citric acid as a precursor. The use of microbial fermentation and the valorization of waste materials will accelerate the transition towards a more sustainable and environmentally friendly approach to CDs production.

In the present work, we show the synthesis, characterization and preliminary applications of green/red absorbing nitrogen-doped CDs (N-CDots). N-CDots were synthesized by one-step autoclave/microwave assisted solvotermal method starting from citric acid and urea. AFM, and FT-IR analysis confirmed the nature of the N-CDots. UV-Vis absorption and photoluminescence spectra showed that optical properties of N-CDots can be tuned over the visible spectrum by simple modifications of synthetic conditions.

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References

[1] X. Xu, R.Ray, et al. *J. Am. Chem. Soc.* **2004**, 126, 40, 12736–12737.
[2] M. Havrdova, K. Hola, et al., *Carbon*, **2016**, *99*, 238-248.
[3] R. M. S. Sendão, J. C.G. Esteves Da Silva, et al., *Catalysts* **2023**, *13*, 179.
[4] E.A. Stepanidenko, E.V. Ushakova et al., *Nanomaterials*, **2021**, *11*, 364.
[5] E. Kou, Y.Yao et al., *ACS Sustainable Chem. Eng*. **2021**, *9*, 944−953.
[6] L.Zhu, L.Chen et al., *Plants* **2022**, *11*, 511.

P 3.19

Perovskite Solar Cells Investigation using A Kinetic Photoconductivity Method

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Fossil fuels, like oil, are still one of the main sources of energy, and the rising prices of fossil fuels encourages the search for alternative energy sources to supply growing energy demand. Photovoltaic systems are one of the most promising types of renewable energy sources, and with the suitable development of photovoltaic systems, it is possible to supply the society's energy needs without fossil fuels fully [1]. Perovskite solar cells, which have attracted a huge scienfic and industrial interest over the past decade, achieved record efficiencies (3.8% to 26.1%) [2]. Perovskite solar cells have a simple technology of manufacturing and can be constructed on the top of other solar cells (Silicon SC, CIGS SC) to obtain more efficient tandem solar cells. This type of solar cells enables the absorption of a wider range of light, thus achieving higher efficiency. The efficiency of tandem solar cells, which has reached a record of 33.7% [2], has been achieved through the use of self-assembled monolayers materials (SAM), which are attracting increasing interest of scientists and companies around the world for the simple methods of formation and cost-effective construction of solar cells [3]. However, there are a lack of data at the movement about self-assembled monolayers materials charge carrier, which determines the efficiency of solar cells. Wider self-assembled monolayers materials investigation would allow specific selection of materials and creation of more efficient perovskite solar cells.

In this work, inverted structure Cs/MA/FA perovskite solar cell, with different SAMs: 2PACz, MeO-2PACz, and polymer PEDOT:PSS was investigated . The goal was, by using photoconductivity measurement method, to see how the charge carrier dynamics of the solar cell is affected by the intensity of light shining on the solar cell as well as effect of the applied external voltage on the solar cell, and how does this dynamic differ when different HTL layers are used.

References

[1] J. S. Shaikh, N. S. Shaikh, A. D. Sheikh, S. S. Mali, A. J. Kale, P. Kanjanaboos, C. K. Hong, J. H. Kim, P. S. Patil, Mater. Des. 2017, 136, 54.

[2] https://www.nrel.gov/pv/cell-efficiency.html

[3] A. Al-Ashouri , A. Magomedov , M. Roß , M. Jošt , M. Talaikis , G. Chistiakova , T. Bertram , J. A. Márquez , E. Köhnen , E. Kasparavičius , S. Levcenco , L. Gil-Escrig , C. J. Hages , R. Schlatmann , B. Rech , T. Malinauskas , T. Unold , C. A. Kaufmann , L. Korte , G. Niaura , V. Getautis and S. Albrecht , Energy Environ. Sci., 2019, 12 , 3356 — 3369

P 3.20

Development of Water-Soluble Semiconducting Polar Polymers for Smart Applications

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The development of new materials is pivotal for the exploitation of the new technologies. One important class of emerging semiconducting materials is represented by conjugated polyelectrolytes (CPEs) comprising an electronically delocalized π-conjugated backbone with pendant groups bearing polar or ionic functionalities [1]. The use of conjugated polyelectrolytes (CPEs) as interfacial layers (ILs) to increase the efficiency of organic light-emitting diodes (OLEDs) [2], organic solar cells (OSCs)[3], [4], and organic transistors is a well-established strategy [5-6].

Structurally, CPEs are generally composed of: (i) π-conjugated backbones, which determine the main optical properties, such as absorption and emission spectra, light-harvesting ability, and quantum yield; (ii) charged side-chains, such as cationic quaternary ammonium groups, anionic carboxyl groups, sulfonic groups, and phosphate groups. CPEs combine the typical properties of polymeric semiconductors, such as chemical tunability, easy processability, lightness and flexibility with the growing demand for environmentally friendly materials. In fact, the incorporation of polar/ionic side groups increases the solubility in water and alcohols, which can potentially endow a more environmentally friendly manufacturing options and increased biocompatibility for sensor applications.

One of the main problems to be addressed is the modification of the polymerization conditions, and purification traditionally carried out under dry conditions and non-aqueous solvents, which must be compatible with polar polymers. The materials obtained must also have a degree of purity suitable for bioelectronic applications.

The commonly employed reactions for the synthesis of CPEs are palladium-catalysed coupling reactions (Suzuki, Heck and Sonogashira), Wessling reaction and $FeCl_3$ oxidative polymerization.

Here we present a series of water/alcohol soluble conjugated polymers synthesized via both ligand free C-H direct arylation and Suzuki Coupling and tested as cathode interfacial layer (CIL) in optoelectronic devices.

References

[1] W. Lee, J. H. Seo, e H. Y. Woo, "Conjugated polyelectrolytes: A new class of semiconducting material for organic electronic devices", *Polymer*, **54**, 5104–5121 (2013)
[2] B. M. Squeo *et al.*, "Benzothiadiazole-based conjugated polyelectrolytes for interfacial engineering in optoelectronic devices", *Pure and Applied Chemistry*, **91**, 477–488 (2019)
[3] Q. Cui e G. C. Bazan, "Narrow Band Gap Conjugated Polyelectrolytes", *Acc. Chem. Res.*, **51**, 202–211 (2018)
[4] E. Lassi *et al.*, "Sulfonate-Conjugated Polyelectrolytes as Anode Interfacial Layers in Inverted Organic Solar Cells", *Molecules*, **26**, 763 (2021)
[5] T. Nguyen-Dang *et al.*, "Dual-Mode Organic Electrochemical Transistors Based on Self-Doped Conjugated Polyelectrolytes for Reconfigurable Electronics", *Advanced Materials*, **34,** 2270170 (2022)
[6] M. Prosa *et al.*, "Organic Light-Emitting Transistors with Simultaneous Enhancement of Optical Power and External Quantum Efficiency via Conjugated Polar Polymer Interlayers", *ACS Appl. Mater. Interfaces*, **10,** 25580–25588 (2018)

P 3.21

Flicker noise analysis shows unusual oligoyne wire features

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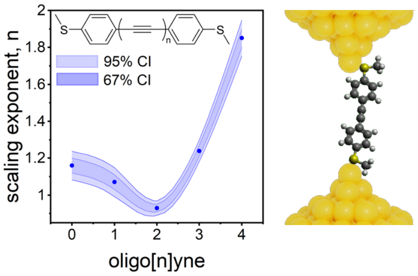
Over the past 8 years, flicker noise analysis has provided an experimental method for determining the coherent tunnelling charge transport pathways in single-molecule junctions. Such pathways are characterised by their relative spatial wavefunction overlap, ranging from poor to strong overlap. The extremes of this range being commonly classified into ‘through-space’ and ‘through-bond’ transport respectively. The method involves evaluating the scaling exponent, n, of the observed power law between the integrated flicker noise, known as the noise power (NP) and the average junction conductance (G_{AVG}), given by $NP \propto G_{AVG}^{n}$. For ‘through-bond’ transport, n is close to 1. Whereas, for ‘through-space’ transport, n is close to 2.

We used this method on a series of thioanisole terminated oligoyne molecular wires. This class of molecular wires is known for their low β values, the tunnelling decay constant across the series, granting long-range coherent transport. In doing so, we have found that the spatial overlap of the scattering state changes across the series. With the scaling exponent initially decreasing with molecular length, before rising again after reaching a minimum, with near-perfect ‘through-bond’ transport observed in the butadiynyl compound.

Such an observation indicates a complex interplay between the competing effects of increased backbone conjugation length and decreased electrode-molecule hybridisation as the molecular length is increased, along with participation to charge transport of non-frontier orbitals. The results of such studies into the determination of n for oligomeric series may lead to a greater understanding of charge transport mechanisms across archetypal molecular wires, beyond simple β-value studies.



The flicker noise scaling exponent, n, versus the oligoyne unit number. 67 and 95 percent confidence intervals for n displayed as dark and light blue bands (left). Single-molecule ethynyl junction (right).

References

[1] Adak, O.; Rosenthal, E.; Meisner, J.; Andrade, E. F.; Pasupathy, A. N.; Nuckolls, C.; Hybertsen, M. S.; Venkataraman, L., Nano Lett., **2015**, 15 (6), 4143–4149.
[2] Wang, C.; Batsanov, A. S.; Bryce, M. R.; Martín, S.; Nichols, R. J.; Higgins, S. J.; García-Suárez, V. M.; Lambert, C. J., J. Am. Chem. Soc., **2009**, 131 (43), 15647–15654.
[3] Naher, M.; Milan, D. C.; Al-Owaedi, O. A.; Planje, I. J.; Bock, S.; Hurtado-Gallego, J.; Bastante, P.; Abd Dawood, Z. M.; Rincón-García, L.; Rubio-Bollinger, G.; Higgins, S. J.; Agraït, N.; Lambert, C. J.; Nichols, R. J.; Low, P. J., J. Am. Chem. Soc., **2021**, 143 (10), 3817–3829.

P 3.22

Semiconducting polymer bio-hybrid interfaces: characterization and first applications

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Keywords: Bioelectronics; Conjugated polymer; P3HT; Bio-hybrid opto-electrical interface; Characterization; Biocompatibility

Bioelectronics is an emergent multidisciplinary field that combines biology and electronics for theragnostic applications. The use of bio-hybrid interfaces to investigate the electrical activity of living cells *in vitro* is at the forefront of bioelectronics and is becoming crucial in the understanding of the network dynamics of cells population. In this framework, microelectrode array (MEA) technology provides key information about single cells interactions, providing the possibility to bridge knowledge from the single cell activity level up to a more complex biological network made by a cell population [1]. In order to modulate the activity of such population, the use of optical stimulation seems a promising strategy to achieve high spatial control of cells stimulation in a physiological manner. In this regard, organic semiconductive polymers absorbing light in the visible spectrum, such as poly(3-hexylthiophene) (P3HT), represent an extremely promising electronic material. P3HT has gained increasing attention, initially, for photovoltaic applications [2] and then for photoactivable interfaces as a potential interactor with living systems. Thus, its ability to absorb visible light is growing an increasing interest in light-mediated cell modulation and stimulation, which have the advantage of high selectivity and spatial resolution, and low/no invasiveness [3]. Based on these considerations, it is of uttermost importance to characterize P3HT films in general, and specifically for these applications. The aim of this work is to compare the optoelectrical properties of P3HT bio-hybrid interfaces consisting of P3HT deposited on ITO glass substrates via spray coating technique, at three different concentrations (2, 5, 10 mg/ml solved in chlorobenzene) and select the best films to be used for the optoelectrical stimulation of a neuronal population. Here, the P3HT sprayed films are characterized by considering morphology and optoelectrical properties, while the morphological properties are evaluated through atomic force microscopy. The optoelectrical properties are measured using a potentiostat and a LED light source (λ = 450, 520, 620 nm). The interchange of a dark phase (10 s) and a phase of light exposition (10 s) is used for the induction of photocurrent (Imax = 2.27 uA at the light ON), measured through the chronoamperometry, and the induction of photovoltage (Vmax= -15 mV at the light ON), measured through the chronopotentiometry. The obtained results show the ability of the polymer to respond to a specific wavelength of light in the visible spectrum (520 nm) and give the possibility to select the best concentration (2 mg/ml) of the polymer for the interaction with *in vitro* biological systems, thus for optimal bio-hybrid interface. Biocompatibility of the spray-coated semiconductive polymer is verified *in vitro* by measuring the growth curves of SH-SY5Y cells at three different time points (24, 48, and 72h) and is estimated to be doubled between the 24 and the 72 hours. The selected P3HT film is then sprayed on multiwell MEA plate, used as a bio-hybrid interface for the neuronal population and stimulated through the Lumos optical stimulation system (Axion Biosystem). Also, in this case the interface is able to answer to the optical stimulation with a photovoltage in the order of mV paving the way to future applications of the bio-hybrid interface for biological systems in complex *in vitro* systems.

[1] Blau A, Murr A, Wolff S, Sernagor E, Medini P, Iurilli G, Ziegler C, Benfenati F. Flexible, all-polymer microelectrode arrays for the capture of cardiac and neuronal signals. Biomaterials. 2011 Mar;32(7):1778-86. doi: 10.1016/j.biomaterials.2010.11.014. Epub 2010 Dec 9. PMID: 21145588.

[2] Holliday, S., Ashraf, R., Wadsworth, A. *et al.* High-efficiency and air-stable P3HT-based polymer solar cells with a new non-fullerene acceptor. *Nat Commun* **7**, 11585 (2016)

[3] Hopkins, J., Travaglini, L., Lauto, A., Cramer, T., Fraboni, B., Seidel, J., & Mawad, D. (2019). Photoactive organic substrates for cell stimulation : progress and perspectives. *Advanced Materials Technologies*, *4*(5). https://doi.org/10.1002/admt.201800744

P 3.23

Accurate Mobility Extraction and Bias Stress Control via Novel Dual-Gate Four-Point-Probe Architecture

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Nowadays, many high-performance organic semiconductors have been reported, some of which even exhibit field-effect mobilities of 10 cm-2 V-1 s-1 or higher. However, the reported mobilities are sometimes overestimated, which is related to the mobility extraction method of organic field effect transistor (OFET).[1] One of the promising ways to measure mobility accurately is four-point-probe measurements.[2] In addition, operational instability is another issue for polymer FETs, which disrupts device functioning in display and electronics applications. Therefore, our project aims to fabricate a polymer FET with real high mobility and excellent operational stability. Here we design a novel dual-gate four-point-probe OFET architecture to extract mobility accurately and control the bias stress measurement process. The bottom gate can be used to fine control the processes happening in the back channel interface, thereby modulating the channel potential during bias stress measurement. This structure can also be used to study the importance of the back channel for the extracted mobility.

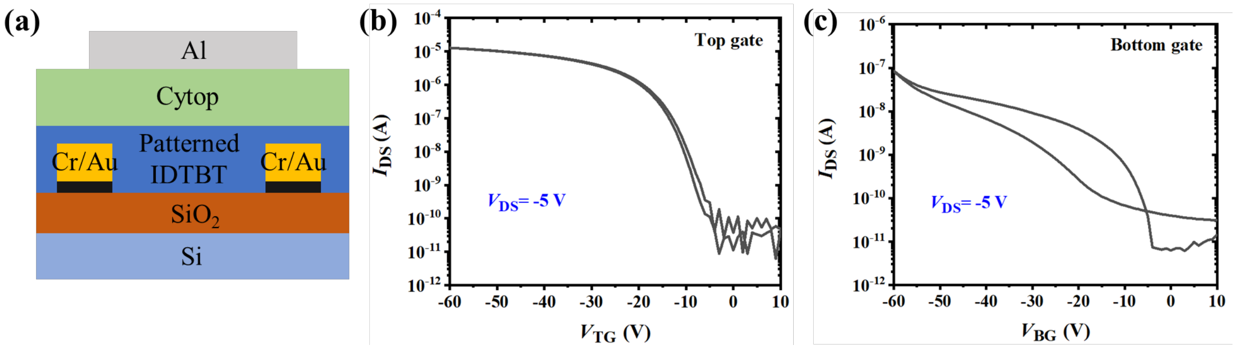

Figure 1. Architecture and device characteristics of dual-gate four-point-probe OFET. (a) Schematic diagram. (b) and (c) show the transfer characteristics of the top and bottom channels, measured separately, respectively.

References

[1] Hu, P., He, X., & Jiang, H. (2021). Greater than 10 cm^2 V^{-1} s^{-1}: A breakthrough of organic semiconductors for field-effect transistors. InfoMat, 3(6), 613-630.
[2] Choi, H. H., Cho, K., Frisbie, C. D., Sirringhaus, H., & Podzorov, V. (2018). Critical assessment of charge mobility extraction in FETs. Nature materials, 17(1), 2-7.

P 3.24

π-Conjugated Food Derived Dyes for Artificial Retinas

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The eye's retina consists of tri-color photoreceptive cones responsible for color vision, detecting short wavelength blue, medium wavelength green, and long wavelength red light with peak absorption at λ=437 nm, λ=533 nm, and λ=564 nm, respectively [1]. Additionally, the rods within the retina are extremely sensitive to low light intensities and contribute to night vision, peaking at 498 nm [2]. Retinitis pigmentosa (RP) and age-related macular degeneration (AMD) are medical conditions that can cause visual impairment [3], due to rods and cones degradation, respectively. Photoactive pixelated retinal prostheses, utilizing food derived π-conjugated chromophore dyes, could be used to elicit neural activity through excitation by careful selection of the π-conjugated small molecules representing the absorption spectra of the photoreceptors of the human eye [4]. Electrolytic photo-capacitor devices (Fig.1) with a typical glass/indium tin oxide (ITO)| titanium oxide (TiO_2)| chromophore dye| biological electrolyte (phosphate buffered saline, PBS) solution| counter electrode structure is reported in this work and investigated via absorption spectra, photocurrent spectra, and transient measurements. Absorption spectra of chromophores were found to be in the visible part of the spectrum, with chlorophyll derived from spinach peaking at 440 nm, and with anthocyanin and betalain chromophore peaks at around 520 nm. The photocurrent spectral response of the samples was correlated with that of absorption; however, some spectral shifts were observed. Photo-current and voltage response signals were clearly evident for all samples, with magnitude from few tens to hundreds of A/m$^{\wedge 2}$ when exposed to pulsed light flash cycles with a pulse length of 20 ms with a 200 ms period using LEDs as excitation sources with emission wavelength close to the peak of the absorption. These findings suggest that the addition of food derived chromophores may be a more environmentally friendly alternative to synthetic dyes. Future research to investigate the effect of other chromophore dyes is needed to realize a fully functional artificial retina.

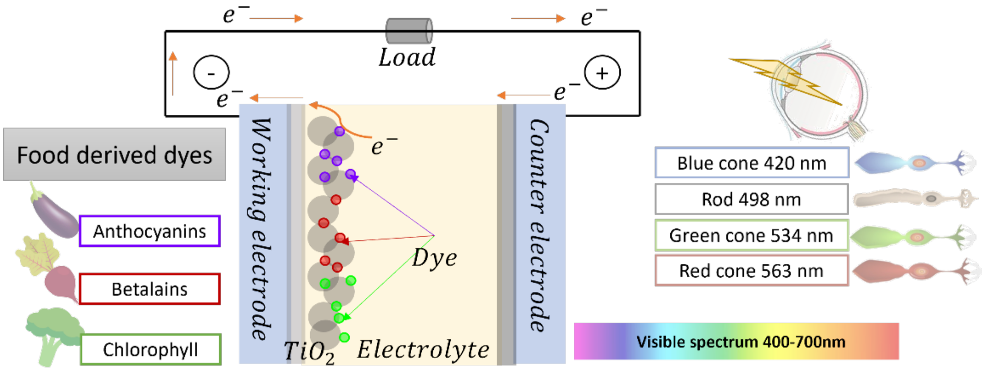

Figure 1 Food derived dyes to mimic the response of rods and cones in artificial retinas.

References

[1] J. K. Bowmaker and H. J. Dartnall, "Visual pigments of rods and cones in a human retina.," *J Physiol*, vol. 298, no. 1, pp. 501–511, 1980, doi: 10.1113/jphysiol.1980.sp013097.
[2] M. Ciocca *et al.*, "Colour-sensitive conjugated polymer inkjet-printed pixelated artificial retina model studied via a bio-hybrid photovoltaic device," *Sci Rep*, vol. 10, no. 1, 2020, doi: 10.1038/s41598-020-77819-z.
[3] L. Askew, A. Sweeney, and M. Shkunov, "Development of polymeric blue prosthetic retina photoreceptors," *MRS Adv*, vol. 8, no. 5, pp. 152–160, May 2023, doi: 10.1557/s43580-023-00525-1.
[4] M. Skhunov *et al.*, "Pixelated full-colour small molecule semiconductor devices towards artificial retinas," *J Mater Chem C Mater*, vol. 9, no. 18, pp. 5858–5867, 2021, doi: 10.1039/d0tc05383j.

P 3.25

Understanding the Surface Chemistry of SnO2 Nanoparticles for High Performance and Stable Organic Solar Cells

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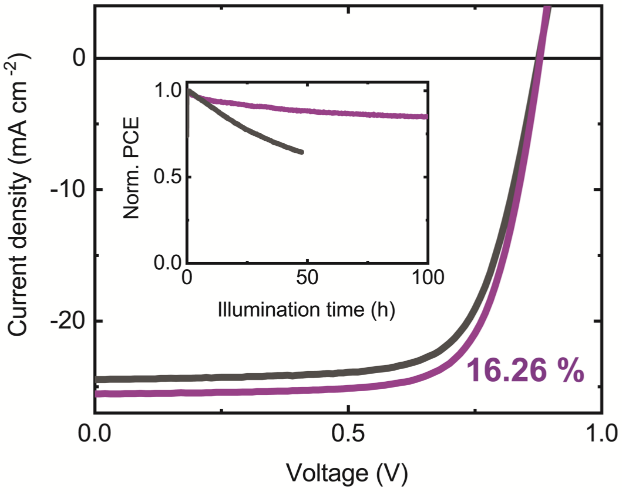
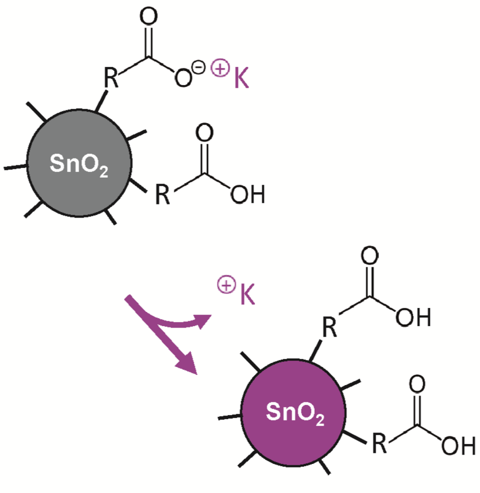
In organic solar cells, the interface between the photoactive layer and the transport layers influences severely the device performance and stability. In particular, when solution-processed metal oxides are employed as the electron transport layer, the presence of surface defects can downgrade the charge extraction, and understanding their origin is essential to mitigate its effect. Herein, we show that a widely reported and commercially available colloidal SnO_2 dispersion leads to a suboptimal interface with the organic layer, as evidenced by the s-shaped J-V curves and poor device stability. By investigating the surface chemistry of the nanoparticles, we identify the presence of potassium ions as stabilizing ligands. By removing them with a simple washing with deionized water, we remove the s-shape and improve short-circuit current. We tested it for two commonly reported blends, TPD-3F:IT-4F and PM6:L8:BO, and for both the power conversion efficiency improved up to 12.82% and 16.26%, from 11.06% and 15.17% obtained with the pristine SnO2, respectively. More strikingly, the stability is strongly correlated with the surface ions concentration, and our improved devices maintain ~87% and ~85% of their initial efficiency after 100h of illumination for TPD-3F:IT-4F and PM6:L8:BO, respectively.





P 3.26

Machine Learning-Accelerated Multiscale Simulations of Redox-Active Polymers for All-Organic Energy Storage

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Polymers with electronic and ionic functionalities present unique possibilities for applications in stretchable electronics, biomedical sensors, and all-organic batteries. The rational design of polymers with specific electronic properties is complicated by their multiscale nature, wherein the interplay between electronic and structural aspects spans a broad spectrum of spatial and temporal scales. This interplay necessitates the inclusion of quantum mechanical descriptions at mesoscopic scales to accurately predict the polymers' electronic functionalities. Consequently, it is essential to devise computational techniques that efficiently combine both mesoscale morphological structures and electronic features.

We introduce an effective computational strategy that combines molecular simulations and machine learning techniques to incorporate electronic structure information at coarse-grained scales [1]. To illustrate, we focus on nonconjugated radical-containing polymers, an emerging class of materials for solid-state organic batteries that rely on pendant redox-active radical sites to transport charge carriers [2]. The use of a coarse-grained model enables the exploration of relevant polymeric length and time scales. At the same time, electronic structure information is retained, enabling trained machine learning models to rapidly predict electronic properties based on the coarse-grained polymer structures. This approach allows to obtain relationships between electronic properties and material morphology, along with processing conditions. We compare our approach to the conventional methodology that involves the conversion of the coarse-grained morphology to atomistic resolution, so-called backmapping, followed by quantum chemical computations, revealing that our approach retains very good accuracy while achieving orders of magnitude speedups. As such, the proposed method holds substantial potential in accelerating multiscale modeling workflows that aim to bridge the quantum and mesoscopic scales in the modeling of polymers with electronic and ionic functionalities.

References

[1] R. Alessandri and J. J. de Pablo, "Prediction of Electronic Properties of Radical-Containing Polymers at Coarse-Grained Resolutions", Macromolecules **2023**, *56*, 3574–3584.

[2] T. Ma, A. D. Easley, R. M. Thakur, K. T. Mohanty, C. Wang and J. L. Lutkenhaus, "Nonconjugated Redox-Active Polymers: Electron Transfer Mechanisms, Energy Storage, and Chemical Versatility", Annual Review of Chemical and Biomolecular Engineering **2023**, *14*, 187–216.

P 3.27

Extraction of force-distance curves in amplitude modulation atomic force microscopy

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The accurate quantification of tip-sample interaction forces in amplitude modulation atomic force microscopy (AM-AFM) has been a challenging yet crucial objective for nanoscale imaging to measure the mechanical properties of biological samples.

This research involves the modeling of force-distance curves in amplitude modulation AFM (also known as "tapping mode"). The approach involves recording amplitude and phase curves as a function of distance and subsequently reconstructing the tip-sample force versus actual tip-sample distance[1]. Analytical formulas are applied to these datasets to calculate the tip-sample force at various tip-sample distances. To validate the method, we conducted numerical simulations that demonstrated the algorithm's reliability by showing agreement between assumed tip-sample interaction models and the reconstructed interaction curves.

Preliminary experiments were performed to reconstruct interaction forces on gold surfaces biofunctionalized with IgM proteins. The force-distance curves will be used to measure the mechanical properties of protein films. This information is relevant for the characterization of biofunctionalized interfaces employed in state-of-the-art large area single-molecule sensors [2].

References

[1] H. Hölscher, ‘’Quantitative measurement of tip-sample interactions in amplitude modulation atomic force microscopy”, *Appl. Phys. Lett.*, ***89*** (12) (2006).
[2] E. Macchia, “Large-Area Interfaces for Single-Molecule Label-free Bioelectronic Detection”, Chem. Rev. (2022).

P 3.28

Inducing Overdrive Suppression in Chicken Cardiomyocytes Using Photovoltaic Devices and Multielectrode Arrays

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Cardiomyocytes exhibit rhythmic electrical activity originating from specialized pacemaker cells, leading to periodic contractions of the cardiac muscle. Disturbance of this periodic cardiac rhythm due to heart damage, stress or ischemia may lead to arrhythmic contractions, with possibly severe and life-threatening consequences [1]. However, the heart has various protective mechanisms to stabilize the cardiac rhythm. One of these mechanisms is called overdrive suppression, which is induced when cardiac tissue is depolarized at frequencies higher than its intrinsic beating rate [2]. The rapid stimulation overwhelms the electrical signaling of the cells, since intra- and extracellular ionic concentrations cannot return to normal levels between stimuli, leading to a momentary pause in the electrical activity [2]. It has been shown that different stimulation protocols affect the duration of this pause in activity in cardiac cell aggregates [2], but it is unclear how localized stimulation of the cells in one region affects the synchronized activity in monolayers of cardiac tissue as a whole. Investigating the causes of overdrive suppression may lead to new insights into the mechanisms of cellular excitability and ion channel dynamics.

In our research, we use custom photovoltaic devices based on a bulk heterojunction composite [3,4] and multielectrode arrays (MEAs) to investigate the effects of different stimulation protocols on cardiac tissue. Monolayers of embryonic chicken cardiomyocytes are cultured on the surface of photovoltaic electrodes, which can be used to induce spatially independent electrical charges in the cardiac tissue when stimulated with red light (660 nm) [3]. By varying the intensity and duration of light pulses, we can investigate the effects of different stimulation parameters on the spontaneous beating of the cardiac tissue. Similarly, cardiac monolayers are cultured on MEAs, which allow for localized stimulation as well as measurement of the electrical activity of cardiac cells. The spatiotemporal changes of the periodic contractions can be observed directly under the microscope or by measuring the changes in intracellular calcium concentrations using fluorescence imaging techniques. Video-based image analysis of selected regions of interest may then be used to track and quantify the contractions of the cardiac tissue [5]. By combining these modalities, we can observe the correlation between mechanical, electrical and calcium activity while the cardiac cells are stimulated to exhibit overdrive suppression.

References

[1] Antzelevitch and Burashnikov: Overview of basic mechanisms of cardiac arrhythmia. Cardiac Electrophysiology Clinics. 2011;3(1):23–45.
[2] Kunysz et al.: Overdrive suppression of spontaneously beating Chick Heart Cell Aggregates: Experiment and theory. American Journal of Physiology-Heart and Circulatory Physiology. 1995;269(3).
[3] Schmidt et al.: Light Stimulation of Neurons on Organic Photocapacitors Induces Action Potentials with Millisecond Precision. Adv. Mater. Technol. 2022, 7, 2101159.
[4] Polz et al.: Holistic Equivalent Circuit Model for Capacitive Extracellular Stimulation. Current Directions in Biomedical Engineering, Vol. 8 (Issue 2), pp. 777-780.

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