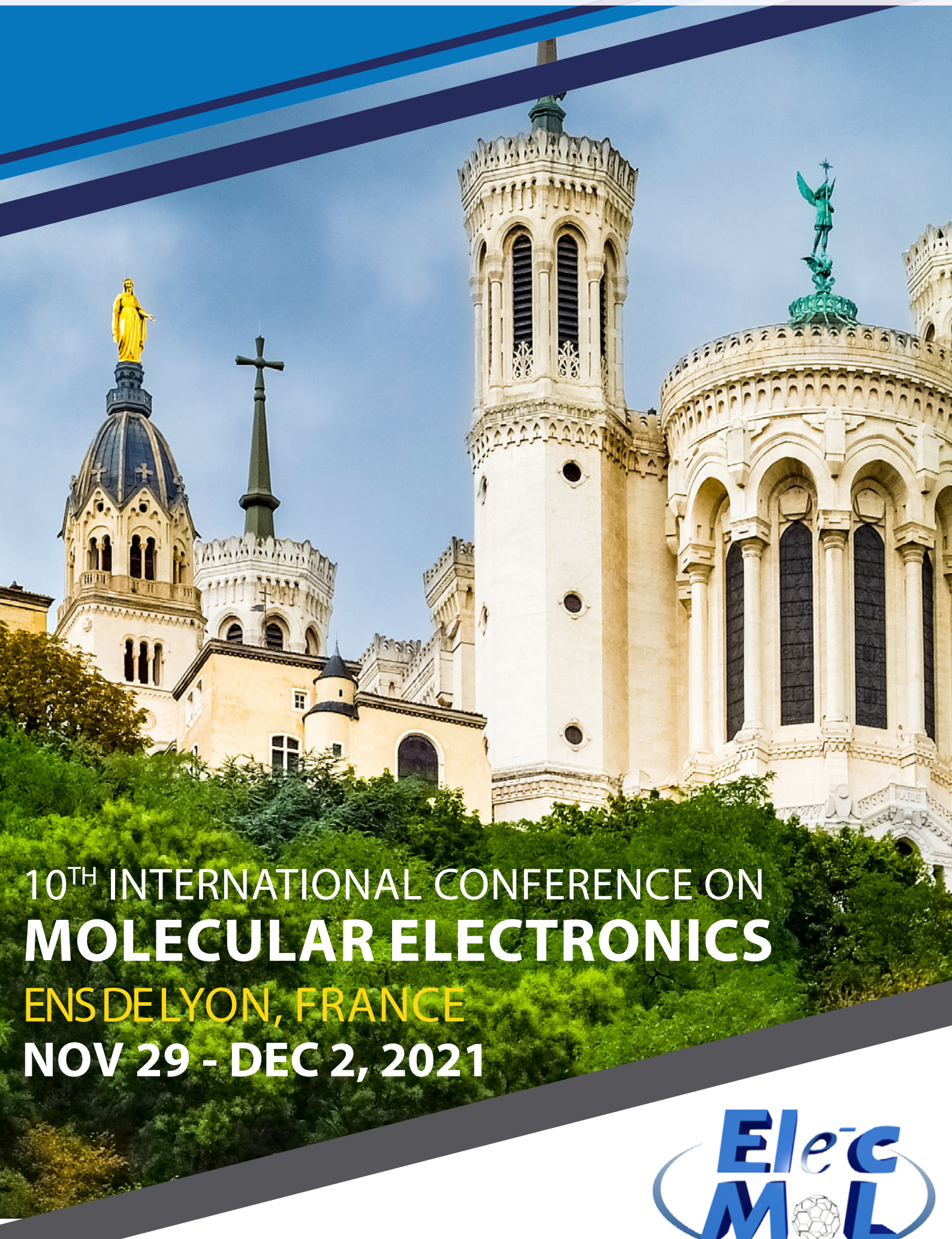
PROGRAM



10TH INTERNATIONAL CONFERENCE ON

MOLECULAR ELECTRONICS

ENS DE LYON, FRANCE

NOV 29 - DEC 2, 2021

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INVITED SPEAKERS

T1 - Single Molecule Junctions, Memories & Switches

Prof. Latha. VENKATARAMAN
(Columbia University, USA)

T2 - Large Area Junctions, Memories & Switches

Dr. Dominique VUILLAUME
(CNRS/Université de Lille, FR)

Prof. Tahkee LEE
(Seoul National University, KR)

T3 - Organic Electronics, Optoelectronics & Photonics

Prof. Koen VANDEWAL
(Hasselt University, BEL)

Prof. Chihaya ADACHI
(Kyushu University, JP)

T4 - 2D materials, Nanotubes & Nanowires

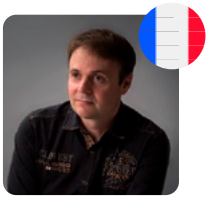
Prof. Alberto MORPURGO
(Université de Genève, CH)

Prof. Katharina J. FRANKE
(Freie Universität Berlin, GER)

INVITED SPEAKERS

T5 - Self-Assembly & Supramolecular Architectures

Prof. Harry L. ANDERSON
(University of Oxford, UK)



Prof. Nicolas GIUSEPPONE
(Université de Strasbourg, FR)

T6 - Scanning Probe Microscopies & Near Field Approaches

Prof. Franz J. GIEßIBL
(Universität Regensburg, GER)

Prof. Andreas HEINRICH
(Ewha Womans' University, KR)

T7 - Molecular Theoretical Modelling

Prof. Denis ANDRIENKO
(Max Planck Institut Mainz, GER)

Prof. Abraham NITZAN
(University of Pennsylvania, USA)

T8 - Bioinspired Approaches & Biomimetic Devices

Prof. David CAHEN
(Weizmann Institute of Science, Israel)

PROGAM - DAY 1

Monday, November 29, 2021

10:00 - 13:00	Registration - Main Hall
13:00 - 13:30	Opening session - Amphithéâtre Mérieux
13:30 - 14:15	PL1 - T6 - Franz J. Gießibl - Probing chemical bonds to natural and artificial atoms by atomic force microscopy
14:15 - 14:30	FL1 - T6 - Elie Geagea - Collective radical oligomerisation induced by an STM tip on a silicon surface
14:30 - 14:45	FL2 - T6 - Lihao Guan - On-surface photoswitch from different AZO and DAE derivatives studied by scanning tunneling microscope
14:45 - 15:00	FL3 - T6 - Vibhuti Rai - Towards tunable single molecule photon sources
15:00 - 15:20	OR1 - T1 - Núria Aliaga-Alcalde - A single-molecule electronic transport survey of nanowires based on curcuminoids
15:20 - 15:40	OR2 - T1 - Albert C. Aragonès - Coupling plasmonic trapping and single-molecule junctions
15:40 - 16:00	OR3 - T1 - Edmund Leary - Long-lived charged states in porphyrin nanoribbons
16:00 - 16:20	Coffee break (Main Hall)
16:20 - 17:05	PL2 - T1 - Latha Venkataraman - Quantum Interference in Single-Molecule Circuits
17:05 - 17:20	FL4 - T1 - Julian Skolaut - Electronic Motor Based on Single Tripodal Chiral Molecule
17:20 - 17:40	OR4 - T1 - Xiaonan Sun - Single Molecule Junctions from metal-complex molecules: Long range charge transport, stability and I/V characteristics
17:40 - 18:00	OR5 - T1 - James Thomas - Electron-phonon interactions in weakly coupled single-molecule junctions
18:00 - 18:20	OR6 - T2 - Jean-Christophe Lacroix - Highly efficient photoswitch in diarylethene-based single- and bi-layer molecular junctions
18:20 - 18:40	OR7 - T2 - Xinkai Qiu - Non-volatile Memory in Large-area Junctions Comprising Self-assembled Fused Porphyrins
18:40 - 20:00	Welcome Cocktail (Main Hall)

PROGAM - DAY 2

Tuesday, November 30, 2021

08:30 - 09:15	PL3 - T2 - Takhee Lee - Towards functional high-yield molecular electronic devices
09:15 - 09:35	OR8 - T2 - Martin Bowen - Information encoding and energy harvesting using the ferromagnetic metal/ molecule interface in quantum spintronic vertical nanodevices
09:35 - 09:55	OR9 - T2 - Prudkovsky - Diarylethene self-assembled monolayers on cobalt with high conductance switching ratio for spintronics
09:55 - 10:10	FL5 - T2 - Laurette-Apolline Jerro - Spin-dependent transport through photoswitchable Self Assembled Monolayers
10:10 - 10:15	Sponsors - OrigaLys
10:15 - 11:15	PO1 - P47 - Poster session and coffee break (Main Hall)
11:15 - 12:00	PL4 - T4 - Alberto Morpurgo - Ionic Gating of 2D Semiconductors
12:00 - 12:00	OR10 - T4 - Marc G. Cuxart - Borophenes made easy: Distinct polymorphs and heterostructures
12:20 - 12:40	OR11 - T4 - Jean-François Dayen - Spin crossover/graphene heterostructure based switchable optoelectronic devices
12:40 - 13:00	OR12 - T4 - Andreas K. Hüttel - Magnetic field control of the Franck-Condon coupling of few-electron quantum states
13:00 - 14:30	Lunch break (Restaurant)
14:30 - 15:15	PL5 - T3 - Koen Vandewal - Inter-molecular charge-transfer states for organic opto-electronics
15:15 - 15:35	OR13 - T3 - Ludovic Favereau - Organic chiral radicals with SOMO-HOMO inversion: A new approach to design stable chiral open-shell materials
15:35 - 15:55	OR14 - T3 - Catherine Demengeat - Key features for efficient long-lived room temperature persistent luminescence of organic molecular crystals
15:55 - 16:10	FL6 - T3 - Alexandre Bachelet - Cavity Effect in Low Volage Operating Organic Field Effect Transistors
16:10 - 17:10	PO1 - P47 - Poster session and coffee break (Main Hall)
17:10 - 17:55	PL6 - T5 - Harry L. Anderson - Porphyrin-Based Molecular Wires
17:55 - 18:15	OR15 - T5 - Thomas Zemb - Four modes of electrical conductivity extending over four orders of magnitude observed in extractant based microemulsions
18:15 - 18:30	FL7 - T5 - Troy L. R. Bennett - Multi-Component Self Assembled Molecular Electronic Thin Films – Towards New High Performance Thermoelectronics
18:30 - 18:45	FL8 - T5 - Soussana Azar - Redox-controlled hybridization of electroactive foldamers
18:45 - 19:00	FL9 - T5 - Ludwig Rotsen - DNA Origami Self-Assembly For Lithography

PROGAM - DAY 3

Wednesday, December 1, 2021

08:30 - 09:15	PL7 - T3 - Chihaya Adachi - Operation mechanism of Hyperfluorescence OLEDs
09:15 - 09:35	OR16 - T3 - Olivier Dautel - Hybrid Field Effect Transistor (HFET): A fully covalent transistor with a pi-conjugated organosilica
09:35 - 09:55	OR17 - T3 - Cassandre Quinton - Nanohoop size influence in bridged cyclo-para-phenylenes
09:55 - 10:15	OR18 - T3 - Andrey Kadashchuk - Determination of the Density-of-States in OLED Host Materials using Thermally Stimulated Luminescence
10:15 - 11:15	PO48 - PO94 - Poster session and coffee break (Main Hall)
11:15 - 12:00	PL8 - T4 - Katharina Franke - Single-layer MoS2 on Au(111) as decoupling layer for organic molecules and magnetic adatoms
12:00 - 12:20	OR19 - T4 - Simon Pascal - Quinonediimine ligands: from oligomeric coordination complexes in solution to molecular wires on surfaces
12:20 - 12:40	OR20 - T4 - Gangamallaiah Velpula - Graphene Meets Ionic Liquids: Fermi Level Engineering via Electrostatic Forces
12:40 - 12:55	FL10 - T3 - J. Alejandro de Sousa - Photoluminescence properties of single-walled carbon nanotubes modified with Stable Organic Radicals
12:55 - 13:00	Sponsors - BioLogic
13:00 - 14:30	Lunch break (Restaurant)
14:30 - 15:15	PL9 - T7 - Denis Andrienko - Chemical design rules for non-fullerene acceptors in organic solar cells
15:15 - 15:35	OR21 - T7 - Cina Foroutan-Nejad - From Memristor to Spinristor; Endohedral Metallofullerenes for Molecular Electronics
15:35 - 15:55	OR22 - T7 - Benoît Champagne - Theoretical Design of Multi-State Multi-Addressable Multi-Functional Molecular Switches
15:55 - 16:10	FL11 - T7 - Sylvain Pitié - Multi-Step Fisher-Lee: A new tool to predict transport mechanism transition in molecular junctions
16:10 - 17:10	PO48 - PO94- Poster session and coffee break (Main Hall)
17:10 - 17:55	PL10 - T8 - David Cahen - Can Protein Electronic Conduction be a Quantum effect?
17:55 - 18:15	OR23 - T8 - Michael Holzinger - Nanostructured Carbon Materials for Bioelectrochemical Applications
18:15 - 18:35	OR24 - T8 - Gareth Redmond - Exploring Memristive Squaraine Nanowire Networks: Programmable Multi-Level Memory Behaviour for Neuromorphic Applications
18:35 - 18:50	FL12 - T8 - Julien Hurtaud - Amyloid fibers for bioelectronics: HET-s(218-289) used for brain-machine interfaces
19:30 - 23:00	Conference dinner at "La Maison"

PROGAM - DAY 4

Thursday, December 2, 2021

08:30 - 09:15	PL11 - T6 - Andreas Heinrich - Electron Spin Resonance of Individual Atomic and Molecular Spins on a Surface
09:15 - 09:35	OR25 - T6 - Benoit Gobaut - Probing local switching currents induced by polarization reversal in an organic ferroelectric thin film
09:35 - 09:55	OR26 - T6 - Anna Rosławska - Light-matter interaction at the single-molecule level probed with STM
09:55 - 10:15	OR27 - T8 - Anne Charrier - Affinity driven ion exchange EG-OFET sensor for high selectivity and low limit of detection of Cesium in seawater
10:15 - 11:15	Coffee break (Main Hall)
10:35 - 11:20	PL12 - T5 - Nicolas Giuseppone - Triarylamine-based Supramolecular Polymers: Structures, Dynamics, and Functions
11:20 - 11:40	OR28 - T5 - Santiago Martin - Building UniMolecular Scaffolding for Electronic Devices
11:40 - 12:00	OR29 - T5 - Henri-Pierre Jacquot de Rouville - Bis-Acridinium Tweezers and Cyclophanes: Supramolecular Self-Assemblies, Self-Sorting and Multi-Switching Properties
12:00 - 12:20	OR30 - T5 - Linghao Yan - Fabrication and Characterization of 2D Metal-Organic Network on Weakly Interacting 2D Materials
12:20 - 12:40	OR31 - T4 - Jean Attias - 2D host–guest supramolecular chemistry for an on-monolayer graphene emitting platform
12:40 - 12:55	FL13 - T2 - Cécile Huez - Redox state-modulated electron transport properties of polyoxometalates at the nanoscale
13:00 - 14:30	Lunch break (Restaurant)
14:30 - 15:15	PL13 - T7 - Abraham Nitzan - Redox molecular junctions and thermal effects
15:15 - 15:35	OR32 - Mikhail Suyetin - Memory Nanodevice Based on Zn-MOF-74: A Molecular Dynamics Study
15:35 - 15:55	OR33 - T7 - Carlo Adamo - Looking for structure/property relations in OPV systems: a multi-level computational approach
15:55 - 16:15	OR34 - T7 - Mariana Kozlowska - Molecular design of semi-conducting metal-organic framework films
16:15 - 16:35	Coffee break (Main Hall)
16:35 - 17:20	PL14 - T2 - Dominique Vuillaume - Electron, spin and thermal transport at the nanoscale in molecular devices: a journey through recent results
17:20 - 18:00	Poster Prize & Closing session - Amphithéâtre Mérieux

Tuesday, November 30, 2021

PO1 - T1 - Lydia Abellan - The role of antiaromaticity in the single molecule conductance of dibenzopentalene compounds
PO2 - T1 - Thomas Baum - Mechanical manipulation of spin-spin interactions in an all-organic di-radical
PO3 - T1 - Hongyan Chen - Indirect Spin-Readout of Rare-Earth-Based Single-Molecule Magnet with STM
PO4 - T1 - Zhixin Chen - Quantum Interference in Graphene-Based Single-Molecule Devices
PO5 - T1 - Jie-Ren Deng - Fused Porphyrin Oligomers for Single-Molecule Electronics
PO6 - T1 - Lukas Gerhard - Influence of electronic environment on molecular light emission
PO7 - T1 - Chunwei Hsu - Substitution Pattern Controlled Quantum Interference in [2.2]Paracyclophane-Based Single-MJs
PO8 - T1 - Karssien Hero Huisman - The CISS effect: A Magnetoresistance Through Inelastic Scattering
PO9 - T1 - Juan Hurtado - Quantum Interference in Radical and Neutral Single-Molecule Junctions
PO10 - T1 - Charlotte Kress - Isocyanides: strong anchoring groups for gold electrodes.
PO11 - T1 - Luca Ornago - Engineering the transport orbital in a molecular junction
PO12 - T1 - L. Palomino Ruiz - 3-state molecular potentiometer based on a non-symmetrically positioned in-backbone linker
PO13 - T1 - Ozlem Sengul - Electrode effects on the observability of destructive quantum interference in single-MJs
PO14 - T1 - S. van der Poel - Mechanically controlled destructive quantum interference in naphthalene based paracyclophanes
PO15 - T2 - S. Al Shehimy - Towards e-triggered Coordination-induced Spin State Switching in Viologen-based Metal Complexe
PO16 - T2 - Pierre Bleteau - Plasmon-Induced Grafting in the Gap of Gold Nanoparticle Dimers for Plasmonic MJs
PO17 - T2 - Camille Jubert Tomasso - Molecular mechanisms involved in organic-based non-volatile memories elucidated through the use of a multiplex platform
PO18 - T2 - J. Lee - Organic Switching Devices processed from Water-Soluble Conductive Polymer and their Characteristics
PO19 - T2 - Bin Lu - Large-area self-assembled gold nanoparticle superlattices for plasmonic and memory devices
PO20 - T2 - Pascal Martin - Formation of organic bi-layers by stepwise electrochemical reduction of diazonium compounds: Bottom-Up Approach
PO21 - T2 - Jacopo Oswald - Graphene-organic semiconductor structures for vertical organic transistors
PO22 - T2 - Margaux Penicaud - Reversible temperature-induced switching in Spin Crossover thin film tunnel junctions
PO23 - T2 - Maryam Sadeghiyan - Growth and multi-scale properties of hybrid magnetic tunnel junctions : towards the control of spinterfaces
PO24 - T2 - Florence Volatron - Switching polyoxometalate monolayers by light irradiation
PO25 - T3 - Ronit S. Bernard - Investigation of carbazole based compounds as electroactive materials for organic electronics
PO26 - T3 - Fatiha Bouihi - Novel hole transporting materials pyrazolopyrimidine and imidazopyrimidine derivatives for perovskite solar cells
PO27 - T3 - Clément Brouillac - New host materials for high performance blue single layer phosphorescent LED
PO28 - T3 - Ozuem Anthony Chukwuka - Matched Rectenna Design Using Organic doped diode for Textile Integration
PO29 - T3 - Roxana Ciorteanu - Optoelectronics properties of some new tetracyclic azaheterocyles
PO30 - T3 - Jesús Alejandro De Sousa Rodríguez - Chiral propeller radical based SAMs
PO31 - T3 - Ranush Durgaryan - Organic small molecules as a hole-transporting materials for efficient perovskite solar cells
PO32 - T3 - Refka El Oueslati - Micro-Mesoporous Conjugated Polymer Based on Poly (Imides-Triazine) as a High-Performance Organic Li-Ion Battery Cathode
PO33 - T3 - Khaoula Ferchichi - Organic doped diode rectifier based on Parylene-electronic beam lithogrpahy process for Radio frequency applications
PO34 - T3 - Sergio Gámez-Valenzuela - Untangling the electronic and charge transport properties of new Naphthalene and Perylene Diimides based-semiconductors
PO35 - T3 - Baptiste Garnier - Prototyping a fully textile rectifier circuit operationg at 13.56 MHz
PO36 - T3 - Etienne Gauthier - Long-lived CPL active chirality-at-rhenium complexes bearing a helicenic NHC ligand: structure-properties relationships to enhance chiroptical & photophysical performances
PO37 - T3 - Przemyslaw Gawel - Multichromophore Systems for Entropy-Driven Singlet Fission
PO38 - T3- Tatiana Ghanem - Direct arylation of push-pull triarylamine dyes based on difluoro-benzothiadiazole units and their evaluation as active material for OPVs
PO39 - T3 - Louis Giraudet - Investigation on organic thin-film transistors by Kelvin Probe Force Microscopy (KPFM)
PO40 - T3 - Nerea G. Pato - Highly fluorescent organic radical molecules arranged into nanoparticles for nanothermometry
PO41 - T3 - Raúl González - Electronic properties of Naphthalimide derivatives
PO42 - T3 - Juozas Vidas Grazulevicius - Derivatives of pyrimidine-5-carbonitrile and carbazole for sky-blue OLEDs and luminescent sensors of oxygen
PO43 - T3 - Claire Guyot - Development of a correlative protocol for depth-resolved chemical analysis of organic LED
PO44 - T3 - Maher Hojorat - Ratiometric Ln3+_based Luminescent Thermometers
PO45 - T3 - Rasa Keruckiene - 3,6-Di-tert-butyl-carbazolyl-disubstituted trifluoromethyl benzene as multifunctional emitter for colour-tuneable OLEDs
PO46 - T3 - Kirill Kondratenko - Correlation between nanoscale thermal and electrical conductivity in PEDOT:OTf thin films
PO47 - T3 - Valentin Lafarge - Study in operando of organic semiconductor stretchability

Wednesday, December 1, 2021

PO48 - T3 - Klaus Leifer - Gas sensors based on nano molecular electronic devices
PO49 - T3 - Simonetti Olivier - Trap characterization in disordered organic semiconductors by Q-DLTS
PO50 - T3 - Eigirdas Skuodis- Synthesis and studies of differently substituted triazatruxenes for organic optoelectronics
PO51 - T3 - Loic Soriano- The defects in the organic spin chain compounds (o-DMTTF)2X (X= Cl, Br and I): a system behaving like a molecular magnet
PO52 - T3 - Ionela Stancu - Electrochemical sensing of naphthalene based on a renewable graphene oxide paste electrode
PO53 - T3 - Joan Teyssandier - Electrical characterizations of individual supramolecular crystals at the local scale
PO54 - T3 - Atul Tripathi - Organic Phototransistor based on oriented thin film of Poly (3- hexylthiophene)
PO55 - T3 - Uliana Tsiko - TADF properties of derivatives of phenothiazine or phenoxazine-substituted benzanthrones emitting in deep-red/near-infrared region
PO56 - T3 - Dmytro Volyniuk- Photophysical and electroluminescent properties of non-planar pyridines ornamented with multiple donor moieties
PO57 - T3 - Wolfgang Weber - Designing ferromagnetic metal/molecule interfaces to preserve molecular functionality
PO58 - T3 - Yuhan Zhong - Controlling the location of dopants in the semi-crystalline structure of oriented thin films of regioregular poly(3-hexylthiophene-2,5-diyl): towards charge conductivities of 3000 S/cm
PO59 - T3 - Walaa Zwaihed - Para-azaquinodimethane: New building block for optoelectronic applications
PO60 - T4 - Idir Achouri - Effect of Cr content on structural, microstructural, magnetic and hyperfine properties of nanostructured (Fe0.7Co0.3)100-xCrx alloys
PO61 - T4 - Haithem Ben Khalifa - Screening of the synthesis route on the structural, magnetic and magnetocaloric properties of La0.6Ca0.2Ba0.2MnO3 manganite
PO62 - T4 - Paul-Gabriel Julliard - Non-covalent assemblies of carbon nanotubes and cobalt corroles applied to ORR
PO63 - T4 - Philippe Lafarge - Hybridization and thermoelectric effects in WSe2 based transistors
PO64 - T4 - Yalan Ma - Probing strain in monolayer MoS2 by scanning tunneling microscopy induced excitonic luminescence
PO65 - T4 - Robin T. K. Schock - Low-temperature transport properties of MoS2 nanotubes
PO66 - T4 - I. Zamkoye- Silver nanowires Electrodes and Plasmon resonance influences on Organic Solar Cell Active Layers
PO67 - T5 - Vivien Andrieux - Electron Responsive Viologen-based Supramolecular Gels
PO68 - T5 - Thaisa B. F. de Moraes - Self-assembly of naphthalene diimide (NDI) within polysilsesquioxane gel
PO69 - T5 - Jean-Luc Bubendorff - A new growth process for crystalline ultra-thin layers of conjugated oligomers used in FETs
PO70 - T5 - Galina Dubacheva - Fluorescence switches based on host/guest interactions: from surfaces to hybrid supramolecular/plasmonic nanostructures
PO71 - T5 - Enrique Escorihuela - 2D array of host-guest complexes as single molecule devices
PO72 - T5 - Raph. Feougier - Hierarchical patterning: sub-10 µm 3D structures nano-textured by block copolymer self-assembly
PO73 - T5 - Tatiana Munteanu - The Substituent Touch upon the Coordination Chemistry of Diamino-benzoquinonediimines
PO74 - T5 - Lionel Patrone - Structural and electrical properties of SAM on Ge as passivating and insulating layers
PO75 - T5 - L. Scarpetta - DAE as functional molecular building blocks to build Electrocatalytic Self-assembled systems for ORR
PO76 - T5 - Z. Tessari - Chirality from scratch: enantioselective adsorption in geometrically controlled lateral nanoconfinement
PO77 - T6 - Frédéric Cherioux - Unravelling the growth mechanism of (3,1) graphene nanoribbons on a Cu(111) surface
PO78 - T6 - Joel Deyerling - On surface synthesis of Por-GNRs on Au(111) and exploration of a new path to decouple molecules from a metallic support
PO79 - T6 - Heigo Ers - The effect of I– addition to the stability of Cd(0001) electrode | RTIL interface
PO80 - T6 - Stéphane Lenfant - Behavior of an Azobenzene Derivative on Gold Exposed to Ultraviolet Light or Electric Field
PO81 - T6 - Christian Wäckerlin - Electronic transport through 1D coordination polymers
PO82 - T7 - Sefia Brahim - Electronic Absorption Spectra Of Platinum (II) Complexes Used For Sensitized Solar Cells
PO83 - T7 - Yannick Dappe - Attenuation Factors in Molecular Electronics: Some Theoretical Concepts
PO84 - T7 - Wenlan Liu - Towards ab-initio accuracy on predicting optical band for organic crystals
PO85 - T7 - Lorenzo Mauro - Charge-transfer chemical reactions in nanofluidic Fabry-Pérot cavities
PO86 - T7 - Giacomo Melani - Donors, acceptors and (a bit of) aromatic: A computational study of molecule-surface interactions onto 2D hexagonal boron nitride towards hybrid electronic interfaces
PO87 - T7 - Justyna Niewiadomska-Kaplar - New approach to the molecular electronics on the example of ethane, ethylene, benzene and acetylene
PO88 - T7 - Saul Sanchez - Relevance of Shockley states on the electrical response of gold-based molecular junctions
PO89 - T7 - Michele Turelli - The role of molecular packing in the optical response of small-molecule OPV materials
PO90 - T7 - Angelo Valli - Local orbitals for ab-initio and many-body simulations of nanoelectronic devices
PO91 - T8 - Karl Griffin - Demonstrating Analog Resistive Switching Behaviour in Squaraine Nanowire Networks
PO92 - T8 - Marine Labro - Synthesis of new photo-generated diazonia derivatives as potential DNA intercalating agents
PO93 - T8 - Kamal Lmimouni - An Electronic Nose with one Single Conducting Polymer? How Mild Doping Tunes P3HT's Chemo Sensitivity for Molecular Recognition
PO94 - T3 - David Kreher - New LC semiconducting (PBTTT)-based polymer : from synthesis to organic FET properties

Invited Speaker

Quantum Interference in Single-Molecule Circuits

Latha Venkataraman

Department of Applied Physics and Chemistry, Columbia University, New York, NY 10027. Email: lv2117@columbia.edu

Abstract:

Over the past decade, there has been tremendous progress in the measurement, modeling and understanding of structure-function relationships in single molecule circuits. Experimental techniques for reliable and reproducible single molecule junction measurements have led, in part, to this progress. In particular, the scanning tunneling microscope-based break-junction technique has enabled rapid, sequential measurement of large numbers of nanoscale junctions allowing a statistical analysis to readily distinguish reproducible characteristics. Although the break-junction technique is mostly used to measure electronic properties of single-molecule circuits, in this talk, I will demonstrate its versatile uses to understand both physical and chemical phenomena with single-molecule precision. I will discuss some recent experimental and analysis aimed at understanding quantum interference in single-molecule junctions. I will then show examples where molecular structures can be designed to utilize interference effects to create a highly non-linear device.

References:

Greenwald et al, Nature Nanotechnology, vol. 16, pages 313–317 (2021).

Invited Speaker

Electron, spin and thermal transport at the nanoscale in molecular devices: a journey through recent results.

Dominique Vuillaume

Institut d'Electronique Microelectronique et Nanotechnologie (IEMN), CNRS, Villeneuve d'Ascq, France.
dominique.vuillaume@iemn.fr

I will review recent results on electron, spin and thermal transport at the nanoscale in molecular self-assembled monolayers (SAMs) and ultra-thin films. These results were mainly obtained by conductive-AFM (in air or UHV) and SThM (scanning thermal microscope) experiments and supported by ab-initio calculations. I will review and discuss:

• the transport properties of polyoxometalates (POMs), which are nano-scaled molecular oxides endowed with a remarkable structural diversity and outstanding magnetic and/or redox properties [1-3].

• the properties of Prussian blue analogs (PBAs) and related cyanide bridged systems, which are coordination networks with unique optical, magnetic, conducting and electrochemical properties [4].

• molecular switches (triggered by light or chemical stimuli) self-assembled on metal and ferromagnetic electrodes with the purpose, in the later case, to develop multifunctional molecular spintronics devices [5-8].

• the thermoelectric properties of organic films and SAMs to assess the role of molecular structures, molecule/electrode interfaces and quantum interferences [9-11].

[1] *Molecular signature of polyoxometalates in electron transport of silicon-based molecular junctions*. Laurans, M.; Dalla Francesca, K.; Volatron, F.; Izzet, G.; Guerin, D.; Vuillaume, D.; Lenfant, S.; Proust, **Nanoscale** *2018*, 10, 17156-17165.

[2] *Charge transport through redox active* $[H_7P_8W_{48}O_{184}]^{33-}$ *polyoxometalates self- assembled onto gold surfaces and gold nanodots.* Dalla Francesca, K.; Lenfant, S.; Laurans, M.; Volatron, F.; Izzet, G.; Humblot, V.; Methivier, C.; Guerin, D.; Proust, A.; Vuillaume, D. **Nanoscale** *2019*, 11, 1863-1878..

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Invited Speaker

Towards functional high-yield molecular electronic devices

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Abstract:

The idea of utilizing individual molecules as the electronic device components has generated a great attention in both understanding the basic transport physics and potential technological applications of molecular electronics [1]. But, fabrication of stable and reliable molecular junctions has been a long-standing challenge in molecular electronics. In this talk, I will review our group's research effort towards fabrication and characterization of high-yield large-scale molecular electronic junctions with device functionalities [2]. Specifically, I will present a series of our experimental advancements to achieve high yield and reliable molecular junctions, such as employing conducting polymer or graphene film as an intermediate electrode layer, or spin-coated reduced graphene oxide layer and directly transferred metals as a top electrode in molecular devices [2,3]. And I will explain the demonstration of molecular junctions with device functionalities such as rectifying, photoswitching, or gated operations [3].

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Invited Speaker

Inter-molecular charge-transfer states for organic opto-electronics

Koen Vandewal[a]

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Abstract:

Charge transfer (CT) states at the interface between electron-donating and electron-accepting (A) materials in organic thin films are characterized by absorption and emission bands within the optical gap of the interfacing materials.[1] Depending on the used donor and acceptor materials, CT states can be very emissive, and/or generate free carriers at high yield.[2] The former can result in rather efficient organic light emitting diodes (OLED), via thermally activated delayed fluorescence, while the latter property is exploited in organic photovoltaic (OPV) devices. In this talk, I will discuss the fundamental properties of CT states and link them to device performance. Furthermore, a new device concept will be introduced, using optical cavity resonance effect enabling narrow-band absorption enhancement,[3] as reduced energy losses in OPV devices.[4]

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Invited Speaker

Operation mechanism of Hyperfluorescence OLEDs

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Chihaya Adachi

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Abstract:

Through the extensive R&D of organic light-emitting diodes (OLEDs) for more than 30 years, plenty of well-elaborated novel organic optoelectronic materials and device architectures have been extensively developed, resulted in the unique commercial utilization of OLEDs for cutting-edge smartphones, large-area TVs, and further new future display applications by taking advantage of light-weight and flexibility. From the aspect of materials science, the creation of novel light-emitting materials in OLEDs has been the central issue aimed for high electroluminescence quantum efficiency (EQE). Starting from the development of conventional fluorescence materials (**1st generation**) during 1990-2000th, the room-temperature phosphorescence (2000-) (**2nd generation**) and thermally activated delayed fluorescence (TADF) (2012-) (**3rd generation**) continuously pioneered the novel possibilities of organic emitters, resulted in not only high-performance OLEDs but also enriched organic photochemistry. In recent days, there have been a wide variety of studies on TADF-OLEDs because of the unlimited possibilities of TADF molecular design. Further, hyperfluorescence (HP)-OLEDs have been developed since they can realize the compatibility of high efficiency and narrow spectral width, which is ideal for practical display applications. Here we report our recent cutting-edge HP-OLEDs demonstrating high OLED performance by optimizing host, TADF, and terminal emitter (TE) molecules[1-3]. In particular, we focus on the blue-emission, which is capable of showing narrow FWHM and high EL quantum yield. Blue HP-OLEDs based on two new TEs are fabricated, resulting in high external quantum efficiency (EQE) of over 20%, high color purity, and high brightness. By analyzing the transient PL characteristics of the HP-OLEDs, we found that the presence of efficient FRET between TADF-assistant dopant (TADF-AD) and TE molecules. Further, transient EL analysis confirmed that a smaller E_{HOMO} difference between TADF-AD and TE efficiently helps to decrease hole trapping inside the emitting layer, hence resulting in a lower efficiency rolloff and a longer operational device lifetime. This report provides a designing principle for a TADF and TE in HP-OLEDs with well-matched energy levels, leading to efficient FRET and no significant carrier trapping.

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Invited Speaker

Porphyrin-Based Molecular Wires

Harry L. Anderson

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Abstract: The synthesis and properties of π-conjugated porphyrin oligomers will be discussed, including charge transport in linear and cyclic porphyrin arrays.

Porphyrins are extremely versatile redox-active π-systems and they are excellent building blocks for the construction of molecular wires.[1-5] This talk will summarize recent work on transport and charge delocalization in porphyrin arrays, such as the butadiyne-linked 12-porphyrin nanoring and the linear edge-fused porphyrin tape shown in Figure 1. The 12-porphyrin ring exhibits global aromatic ring currents in the 6+ and 10+ oxidation states.[3] Charge transport through the linear fused trimer was tested as a function of gate potential, by connecting it across a graphene nanogap.[5]

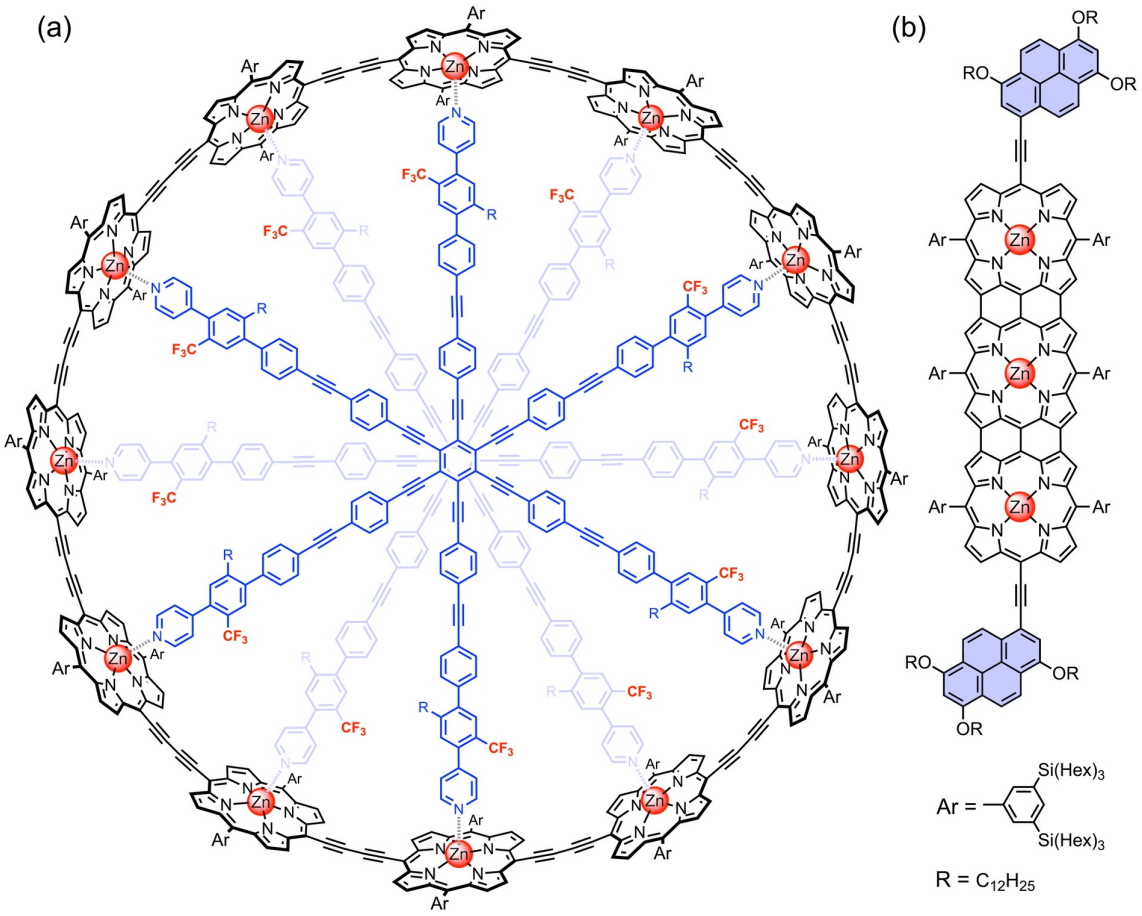

*Figure 1. (a) A cyclic porphyrin dodecamer bound to two molecules of a **T6** template.[3] (b) A fused porphyrin trimer with alkoxypyene anchor groups.[5]*

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Invited Speaker

Ionic Gating of 2D Semiconductors

Alberto Morpurgo,[a]

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Abstract:

Ionic gating exploits electrolytes to control electrostatically the properties of semiconductors, in transistor devices with very large gate capacitance, in excess of 50 $\mu F/cm^2$ (three orders of magnitude larger than the capacitance of a commonly used, 300 nm thick SiO_2 gate dielectric). Such a large capacitance allows charge densities up to 5 10^{14} cm^{-2} to be accumulated at the surface of different semiconductors, and causes new phenomena to appear, among which gate-induced superconductivity is possibly the best-known example. As the level of control and understanding of ionic gating continues to improve, new applications of ionic gated devices emerge. Here I will discuss two aspects. First, I will show how the very large gate capacitance of ionic gated devices allows quantitative energy spectroscopy of band edges in 2D semiconductors, allowing precise measurements of band gaps and band alignment. Second, I will discuss double-gated ionic devices allowing extremely large values of electric field to be applied perpendicularly to atomically thin semiconducting layers, so strong to enable band gaps as large as 1.5 eV to be fully quenched. I will illustrate this result with systematic measurements performed on few layer WSe_2 double gated device, in which we succeeded in quenching the gap of tri-layer and thicker WSe_2 crystals.

Invited Speaker

Single-layer MoS_2 on Au(111) as decoupling layer for organic molecules and magnetic adatoms

Sergey Trishin, Nils Krane, Nils Bogdanoff, Gael Reecht, Christian Lotze, Felix von Oppen, Katharina Franke

Fachbereich Physik, Freie Universität Berlin, Germany

Abstract:

Adsorption of atoms and organic molecules on metal surfaces typically leads to strong hybridization of the frontier molecular orbitals with the substrate electronic bands. This results in broad energy levels reflecting the ultrashort lifetime of excited states in tunneling experiments. A monolayer of MoS_2 is a direct-bandgap semiconductor. Here, we show that single-layer MoS_2 on Au(111) acts as an efficient decoupling layer for organic molecules and magnetic adatoms. Molecular resonances within the semiconducting band gap of MoS_2 exhibit widths of only a few meV. This exquisite energy resolution allows to study vibrational excitations and their spatial variations within the individual molecules [1,2].

Furthermore, we investigate single Fe atoms on MoS_2/Au(111). We find that the decoupling efficiency strongly varies across the moiré pattern induced by the lattice mismatch at the interface. Fe atoms located on the minima of the moiré structure show sharp inelastic spin excitations. In contrast, Fe atoms on the moiré maxima exhibit a Kondo resonance. We track the evolution of magnetic excitations by investigating Fe atoms on different adsorption sites with respect to the moiré pattern and ascribe the gradual increase of Kondo correlations to the moiré-modulated density of states [3].

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Invited Speaker

Probing chemical bonds to natural and artificial atoms by atomic force microscopy

Franz J. Giessibl

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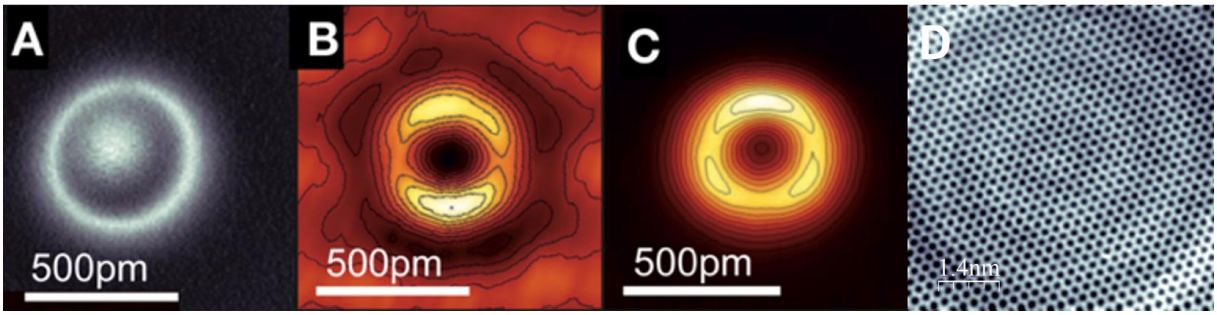
Atomic force microscopy with CO terminated tips has demonstrated outstanding spatial resolution on organic molecules [1], metallic clusters [2] and many other samples. Experimental evidence and calculations show that the CO tip is chemically inert and probes organic molecules mainly by Pauli repulsion [3]. Thus, images of organic molecules, graphene etc. observed with a CO tip can be interpreted as a map of the absolute charge density of the sample. The total charge density of a single adatom is approximately given by a Gaussian peak. While single silicon adatoms appear similar to a Gaussian peak when imaged by AFM with a CO terminated tip, copper and iron adatoms adsorbed on Cu(111) and Cu(110) appear as tori [2,4]. Experiments and DFT calculations show that the total charge density of Cu and Fe adatoms is approximately Gaussian – in contrast to the hybridization theory [4]. The bonding strength between the AFM tip and the atoms of the sample depends not only on the chemical identity but also on the coordination - corner atoms in clusters are more reactive than center atoms [5].

Progress in force resolution [6] opens up the fN-regime, allowing to study engineered surface structures such as quantum corrals that form artificial atoms and interact in a similar way as natural atoms, yet with a force of only 1/1000 of what is experienced in natural atoms [7].



AFM images of various metallic adatoms using a CO terminated tip. **A** *Copper adatom on Cu(111).* **B** *Copper adatom on Cu(110).* **C** *Iron adatom on Cu(111).* **D** *Quantum Corral after Crommie, Lutz and Eigler [8] on Cu(111).*

References:

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Invited Speaker

Electron Spin Resonance of Individual Atomic and Molecular Spins on a Surface

A.J. Heinrich[1,2]

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Abstract:

Scanning Tunneling Microscopy (STM) can be combined with electron spin resonance [1]. The major advantage of spin resonance is the fact that the energy resolution is independent of the temperature and thus can be much higher than a Fermi-function limited spectroscopy technique such as STM tunneling. In ESR-STM we apply a microwave-frequency electric field to the STM tunnel junction and convert this AC electric field into a driving field for the ESR. We find an energy resolution, which is about 10,000 times better than low-temperature STM. Two advantages of ESR-STM over ensemble-averaging techniques are first, the obvious fact that individual spin systems are measured and second, that this can be combined with precise atom manipulation to build engineered nanostructures.

We will begin by introducing the basic concepts of STM, which might be new to some members of this community. Then we will focus on one example of ESR-STM. We will utilize the atomic spin of Ti-H molecules which are adsorbed on thin MgO films supported on Ag metal substrates. Ti-H is a beautiful example since it has a spin of S=1/2 in this configuration together with a rich isotope distribution including nuclear spins [2].

In the second example we will investigate molecules with ESR-STM. We found that Fe-Pc has an S=1/2 spin state due to charge transfer from the substrate. In contrast to Fe atoms on the same surface, this spin is isotropic and shows no signs of magnetic anisotropy [3].

ESR-STM is just in its infancy with many groups joining this research effort. I believe that this technique will occupy a bright corner of quantum-coherent nanoscience.

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Invited Speaker

Chemical design rules for non-fullerene acceptors in organic solar cells

A. Markina,[a] K.-H. Lin,[a] W. Liu,[a] C. Poelking,[a] Y. Firdaus,[b] D. R. Villalva,[b] J. I. Khan,[b] S. H. K. Paleti,[b] G. T. Harrison,[b] J. Gorenflot,[b] W. Zhang,[b] S. De Wolf,[b] I. McCulloch,[b] T. D. Anthopoulos,[b] D. Baran,[b] F. Laquai,[b] D. Andrienko [a]

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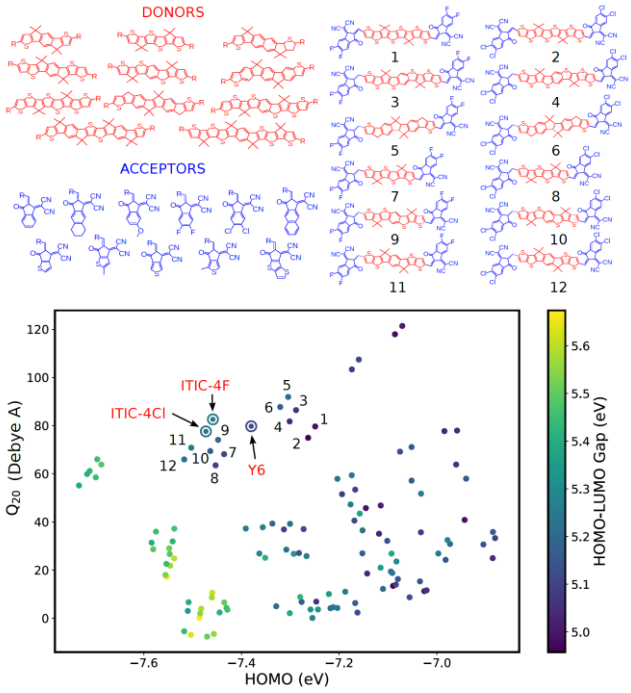
[b] *King Abdullah University of Science and Technology (KAUST), Thuwal, Kingdom of Saudi Arabia*

Abstract:

Efficiencies of organic solar cells have practically doubled since the development of non-fullerene acceptors (NFAs). However, generic chemical design rules for donor-NFA combinations are still needed. We propose such rules by analyzing inhomogeneous electrostatic fields at the donor-acceptor interface. We show that an acceptor-donor-acceptor molecular architecture, and molecular alignment parallel to the interface, result in energy level bending that destabilizes the charge transfer state, thus promoting its dissociation into free charges. By analyzing a series of PCE10:NFA solar cells, with NFAs including Y6, IEICO, and ITIC, as well as their halogenated derivatives, we suggest that the molecular quadrupole moment of ca 75 Debye Angstrom balances the losses in the open circuit voltage and gains in charge generation efficiency.



Left: Chemical structures of acceptors and donors with R depicting the donor-acceptor bonds. Right: Molecular structures of 12 selected compounds. Bottom: Q20-HOMO plot for 121 A-D-A compounds as well as high-performance NFAs ITIC-4F, ITIC-4Cl, and Y6. Each point is colored according to its corresponding HOMO-LUMO gap value. Reprinted with permission from Advanced Energy Materials, 2021

References:

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J. I. Khan, et al, Adv. Energy Mater., 2100839, 2021

Invited Speaker

Triarylamine-based Supramolecular Polymers: Structures, Dynamics, and Functions

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Abstract:

Triarylamine molecules and triarylamine-based covalent polymers have been extensively investigated for more than sixty years in academics and industry because of their intriguing electronic and optical characteristics. However, despite the profusion of studies made on these derivatives, only very recently have the first examples of supramolecular polymers based on the triarylamine motif been described in the literature. Specifically, our research group has shown that, by adding supplementary hydrogen bonding moieties such as amide functions in their periphery, it becomes possible to tightly pack triarylamine molecules in columnar supramolecular stacks presenting a collinear arrangement of their central nitrogen atoms. These supramolecular polymers can self-assemble into various soft hierarchical structures such as helical fibers, nanorods, nanospheres, and nanoribbons in the sol and in the gel states, into liquid-crystalline mesophases, as well as into highly organized supramolecular frameworks and their single crystals thereof. Interestingly, the associated supramolecular polymerization mechanism involves a nucleation step of high activation energy which requires the flattening of the triarylamine core. Because of this singularity, and although dependent on the precise chemical nature of the building blocks, it has been demonstrated that their supramolecular polymerization can be triggered by original tools such as light irradiation or electrochemistry, and that it can display autocatalytic growth behaviors, remarkably strong amplifications of chirality, as well as complex and competing thermodynamic and kinetic self-assembly pathways. Further, from a functional point of view, it has been highlighted that a partial oxidation of the triarylamine molecules results in an enhanced through-space delocalization of the charge carriers along the π-π stacked supramolecular polymers, a feature that confers to these nanowires exceptional transport properties. Upon increasing the charge carrier concentration, the electronic nature of these soft materials can be switched from a semiconducting to a metallic behavior, and the presence of highly delocalized unpaired electrons in supramolecular polaronic band structures has been further exploited to implement plasmonic properties within subwavelength organic interconnects and microscopic optical waveguides. Finally, by making use of the unusual dynamics and functions of triarylamine-based nanostructures, it becomes possible to precisely address their self-construction within confined environments or within nano- and micrometer scale devices. This has been demonstrated for instance in between nanoparticles and in between electrodes, inside inorganic nanopores and inside phospholipid bilayers, as well as at the liquid-liquid interface. Such a meeting point between bottom-up and top-down technologies is of high interest to envision further developments and applications for this entirely new class of supramolecular polymers which combine a unique relationship between their structures, their dynamics, and their subsequent emerging functional properties.

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Moulin, E.; Armao IV, J.; Giuseppone, N. *Acc. Chem. Res*. **2019**, *52*, 975-983.

Invited Speaker

Redox molecular junctions and thermal effects

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Abstract:

Redox molecular junctions are molecular conduction junctions that involve more than one oxidation state of the molecular bridge. This property is derived from the ability of the molecule to transiently localize transmitting electrons. I will discuss the implications of this behavior in a system open to electron flux and their manifestations with regards to the nonlinear transport properties, energy conversion, switching and thermal conduction.

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10th International Conference on Molecular Electronics
November 29 - December 2, 2021

Invited Speaker

Can Protein Electronic Conduction be a Quantum effect?

David Cahen*

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Abstract:

Solid state Electron Transport (ETp), *electronic* conduction, across junctions with an ultra-thin protein film as active layer, can be surprisingly efficient. Length-normalized, ETp efficiency can be similar to, or even exceed that of conjugated molecules; moreover, it can be temperature-independent down to at least 4K. If intra-protein transport dominates, i.e., contacts are not limiting (not straightforward, as proteins are polyelectrolytes), then we cannot measure a significant transport barrier.

Such results have, nowadays, the banner "*quantum*" all over them, as they seem consistent with tunneling; one of the problems with such explanation, apart from the distances involved, is the implied coherence of transport. While coherent transport seems unlikely, the results are surprising, given that

- the system is disordered, and
- in biology electron transfer, ET, via proteins, occurs at *room temperature* in an aqueous electrolyte and/or membranes, and is ion transport-coupled.

Still, understanding ETp may have relevance for ET (replace coupling to the contacts by electron injection/extraction). I will discuss experimental data,[1,2] also from other groups, which help define the puzzle, which we try to solve.[3]

* work done with **Mordechai Sheves and Israel Pecht**, *the Weizmann Institute*
Ayelet Vilan, former students & former and present postdoctoral fellows, *the Weizmann Institute* ;
other collaborations are with Jochen Blumberger (London); Gabor Vattay (Budapest); Carlos Cuevas (Madrid) & Linda Zotti (Sevilla); Marc Tornow (Munich) ; David Lederman (Santa Cruz) +++.

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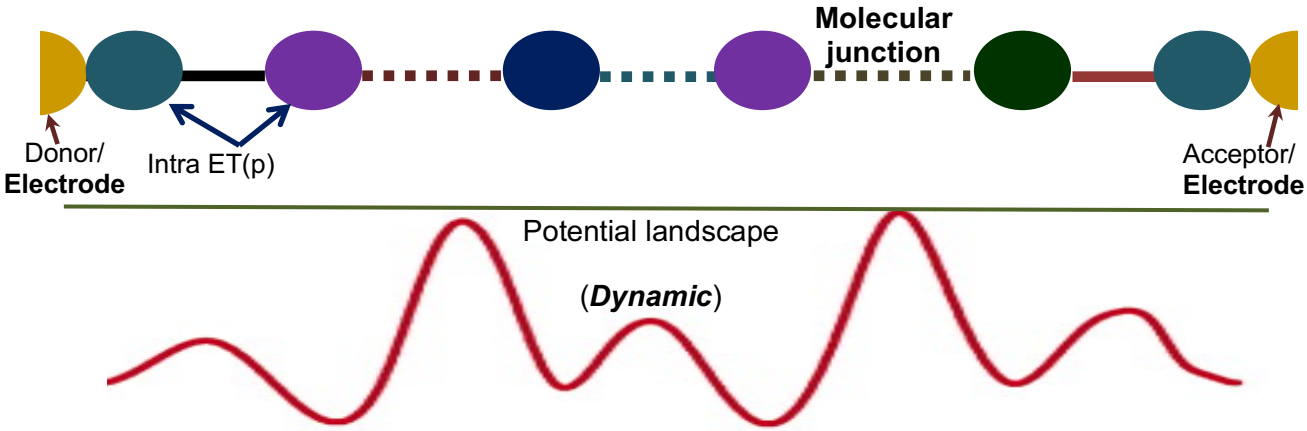

Figure: Schematic of protein junction, depicted as arrangement of amino-acids and cofactors, (TOP) and a snap-shot (< psec) of the electrostatic potential (BOTTOM); from ref. 1, to be referred to as the source.

CONFERENCE SCHEDULE

ELECMOL 2021
10th INTERNATIONAL CONFERENCE ON MOLECULAR ELECTRONICS

NOVEMBER 29 - DECEMBER 2 | 2021

DAY 1
NOV 29 | MON

10:00-13:00
Registration

13:00-13:30
Opening

13:30 14:15	J.-C. LACROIX	GIEßIBL (T6)
14:15 14:30		GEAGEA (T6)
14:30 14:45		GUAN (T6)
14:45 15:00		RAI (T6)
15:00 15:20		ALIAGA (T1)
15:20 15:40		ARAGONES (T1)
15:40 16:00		LEARY (T1)

16:00-16:20
Coffee Break

16:20 17:05	N. ALIAGA	VENKATARAMAN (T1)
17:05 17:20		SKOLAUT (T1)
17:20 17:40		SUN (T1)
17:40 18:00		THOMAS (T1)
18:00 18:20		LACROIX (T2)
18:20 18:40		QIU (T2)

18:40-20:00
Welcome Cocktail

DAY 2
NOV 30 | TUE

08:30 09:15	P. LAFARGE	LEE (T2)
09:15 09:35		BOWEN (T2)
09:35 09:55		PRUDKOVSKY (T2)
09:55 10:10		JERRO (T2)

ORIGALYS TECHNICAL PRESENTATION

10:15-11:15
Poster Session (PO1-PO47)
&
Coffee Break

11:15 12:00	J. CORAUX	MORPURGO (T4)
12:00 12:20		CUXART (T4)
12:20 12:40		DAYEN (T4)
12:40 13:00		HÜTTEL (T4)

13:00-14:30
Lunch Break

14:30 15:15	D. VUILLAUME	VANDEWAL (T3)
15:15 15:35		FAVEREAU (T3)
15:35 15:55		DEMANGEAT (T3)
15:55 16:10		BACHELET (T3)

16:10-17:10
Poster Session (PO1-PO47)
&
Coffee Break

17:10 17:55	J. WEISS	ANDERSON (T5)
17:55 18:15		ZEMB (T5)
18:15 18:30		BENNETT (T5)
18:30 18:45		AZAR (T5)
18:45 19:00		ROTSEN (T5)

DAY 3
DEC 1 | WED

08:30 09:15	K. LEIFER	ADACHI (T3)
09:15 09:35		DAUTEL (T3)
09:35 09:55		QUINTON (T3)
09:55 10:15		KADASHCHUK (T3)

10:15-11:15
Poster Session (PO48-PO94)
&
Coffee Break

11:15 12:00	A.-J. ATTIAS	FRANKE (T4)
12:00 12:20		PASCAL (T4)
12:20 12:40		VELPULA (T4)
12:40 12:55		DE SOUSA (T3)

BIOLOGIC TECHNICAL PRESENTATION

13:00-14:30
Lunch Break

14:30 15:15	C. ADAMO	ANDRIENKO (T7)
15:15 15:35		FAROUTAN-NEJAD (T7)
15:35 15:55		CHAMPAGNE (T7)
15:55 16:10		PITIE (T7)

16:10-17:10
Poster Session (PO48-PO94)
&
Coffee Break

17:10 17:55	K. LMIMOUNI	CAHEN (T8)
17:55 18:15		HOLZINGER (T8)
18:15 18:35		REDMOND (T8)
18:35 18:50		HURTAUD (T8)

19:30-22:30
Conference Dinner

DAY 4
DEC 2 | THU

08:30 09:15	F. CHÉRIOUX	HEINRICH (T6)
09:15 09:35		GOBAUT (T6)
09:35 09:55		ROSLAWSKA (T6)
09:55 10:15		CHARRIER (T8)

10:15-10:35
Coffee Break

10:35 11:20	H. ANDERSON	GIUSEPPONE (T5)
11:20 11:40		MARTIN (T5)
11:40 12:00		J. DE ROUVILLE (T5)
12:00 12:20		YAN (T5)
12:20 12:40		ATTIAS (T4)
12:40 12:55		HUEZ (T2)

HTDS TECHNICAL PRESENTATION

13:00-14:30
Lunch Break

14:30 15:15	E. DUMONT	NITZAN (T7)
15:15 15:35		SUETIN (T7)
15:35 15:55		ADAMO (T7)
15:55 16:15		KOZLOWSKA (T7)

16:15-16:35
Coffee Break

16:35 17:20	C. BUCHER	VUILLAUME (T2)

17:20-18:00
Poster Prize & Closing


Lyon 1
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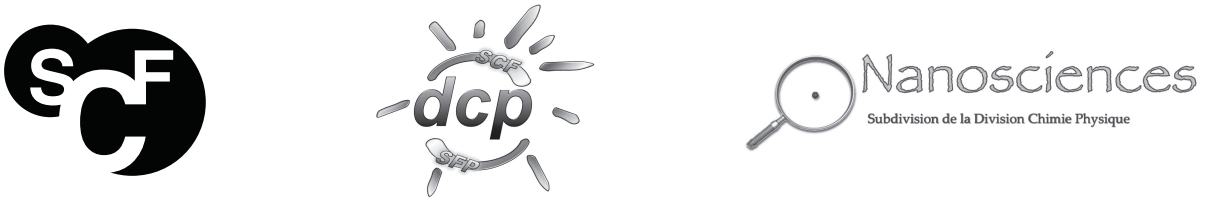
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