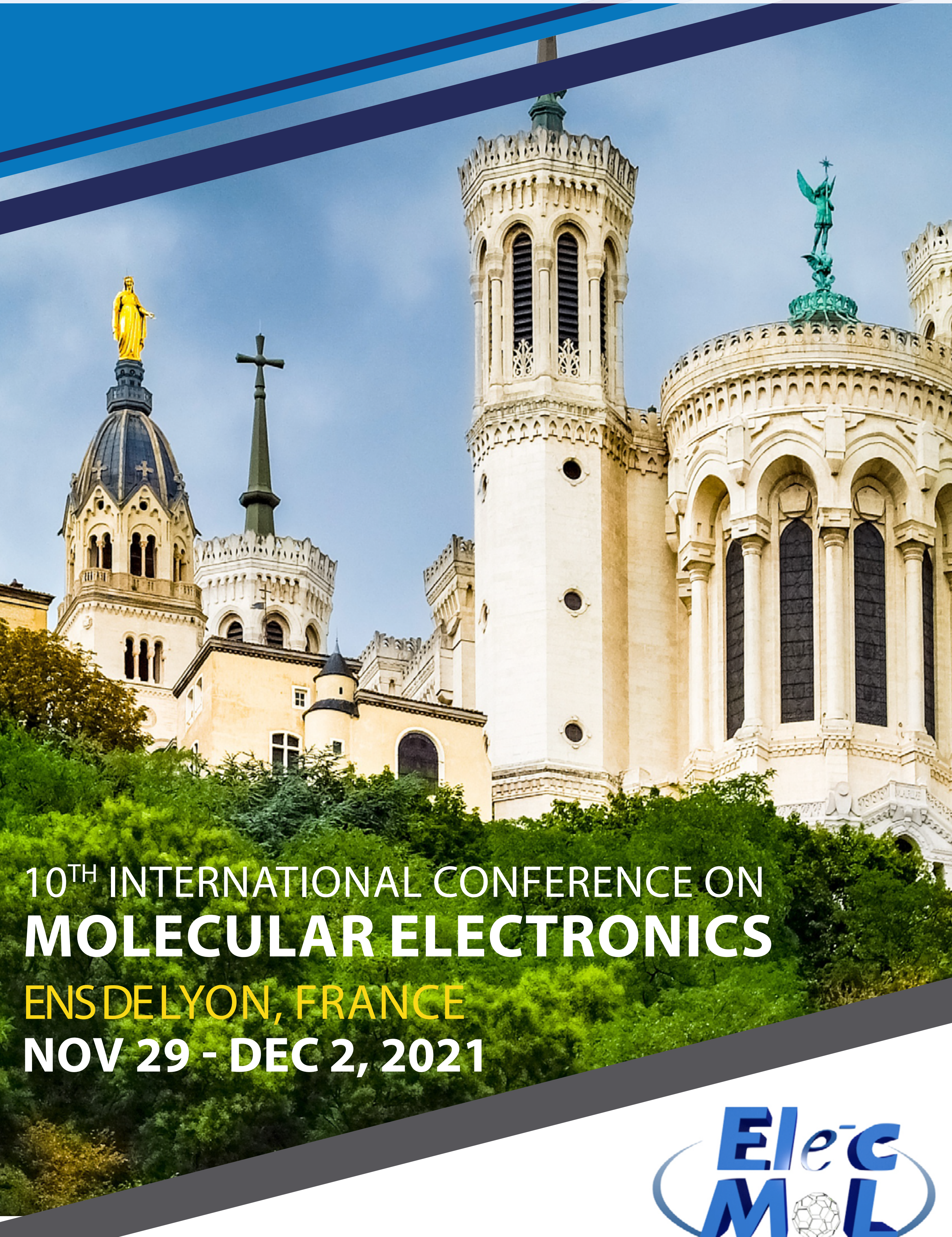
BOOK OF ABSTRACTS



10TH INTERNATIONAL CONFERENCE ON

MOLECULAR ELECTRONICS

ENS DE LYON, FRANCE

NOV 29 - DEC 2, 2021

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INVITED SPEAKERS

Single Molecule Junctions, Memories & Switches

Prof. Latha. VENKATARAMAN
(Columbia University, USA)

Large Area Junctions, Memories & Switches

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

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(Seoul National University, KR)

Organic Electronics, Optoelectronics & Photonics

Prof. Koen VANDEWAL
(Hasselt University, BEL)

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(Kyushu University, JP)

2D materials, Nanotubes & Nanowires

Prof. Alberto MORPURGO
(Université de Genève, CH)

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

INVITED SPEAKERS

Self-Assembly & Supramolecular Architectures

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

Prof. Nicolas GIUSEPPONE
(Université de Strasbourg, FR)

Scanning Probe Microscopies & Near Field Approaches

Prof. Franz J. GIEßIBL
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Molecular Theoretical Modelling

Prof. Denis ANDRIENKO
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(University of Pennsylvania, USA)

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)

Invited Speaker

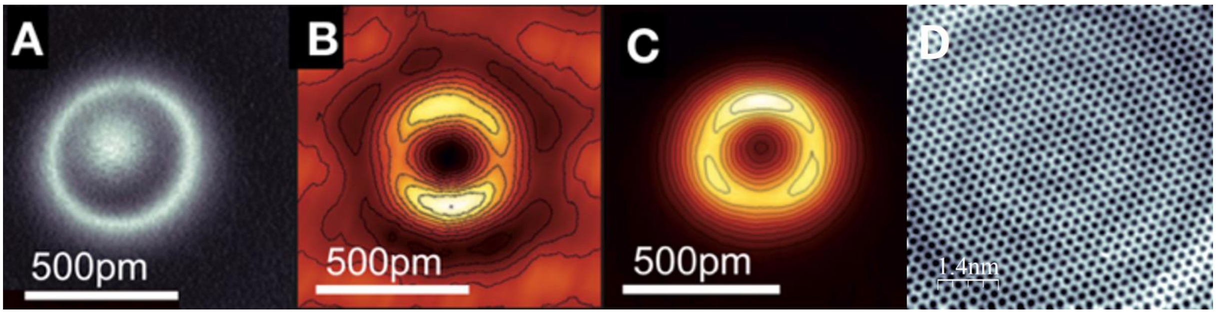
Probing chemical bonds to natural and artificial atoms by atomic force microscopy

Franz J. Giessibl

Chair for Quantum Nanoscience, Institute of Experimental and Applied Physics, University of Regensburg, D-93053 Regensburg, Germany, Email: Franz.Giessibl@ur.de

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:

[1] L. Gross et al., *Science* **325**, 1110 (2009).
[2] M. Emmrich et al., *Science* **348**, 308 (2015).
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[4] F. Huber et al., *Science* **366**, 235 (2019).
[5] J. Berwanger et al., *Phys. Rev. Lett.* **124**, 096001 (2020).
[6] A. Liebig et al., *New Journal of Physics* **22**, 063040 (2020).
[7] F. Stilp, et al., *Science* **372**, 1196 (2021).
[8] M.F. Crommie, C.P. Lutz, D.M. Eigler, *Science* **262**, 218 (1993).

Collective radical oligomerisation induced by an STM tip on a silicon surface

Elie GEAGEA,[a] Judicael JEANNOUTOT,[a] Michel FERON,[a] Frank PALMINO,[a] Alain ROCHEFORT,[b] Christophe M. THOMAS [c] and Frédéric CHERIOUX [a]

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Abstract:

Over the two past decades, on-surface covalent synthesis of organic nanostructures, has been widely investigated in the aim of fabrication of molecular electronic components and functional nanomaterials, owning to the Scanning Tunneling Microscopy monitoring which enhanced the synthesis comprehension at the atomic-scale size precision.[1] Here, we introduce a new strategy to obtain alkyl oligomers in a controlled manner using on-surface radical oligomerisations that are triggered by electrons between the tip of a scanning tunnelling microscope and the Si(111)-B surface (Figure).[2] This electron transfer event only occurs when the bias voltage is below -4.5 V and allows access to reactive radical species under exceptionally mild conditions. This transfer can effectively 'switch on' a sequence leading to the formation of oligomers of defined size distribution due to on-surface confinement of the reactive species. Our approach enables new way to initiate and control radical oligomerisations with tunnelling electrons, leading to molecularly precise nanofabrication.

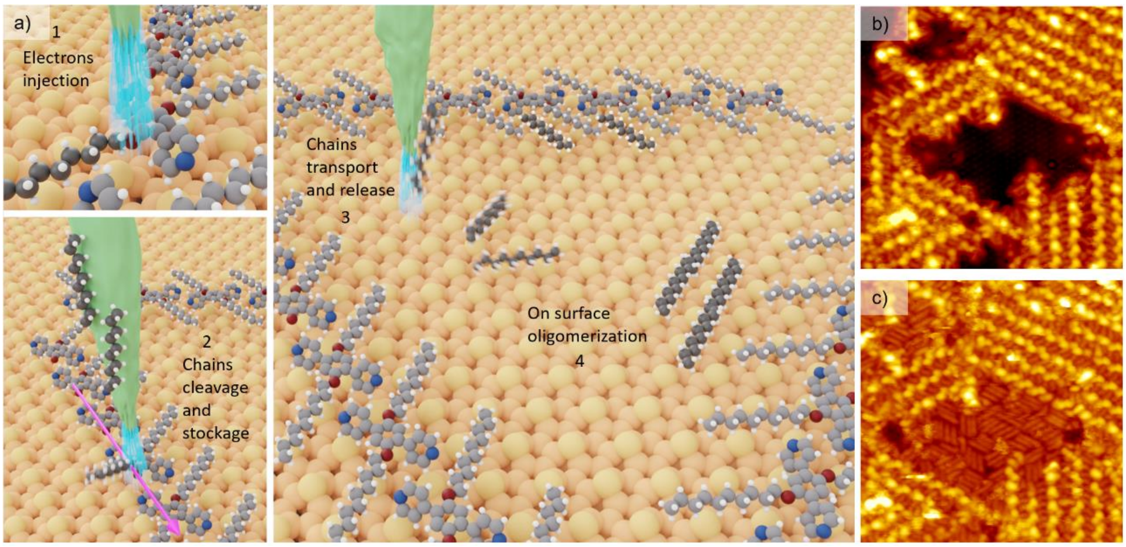

Figure: a) Representative schemes of the new strategy showing the subsequent steps of stm tip induced olygomerisations on Si(111)-B surface. b) STM image (25x25 nm2, Vs = -1.3 V, It = 7 pA, T = 110 K) representing an nano-pore inside the supramolecular network. c) The same nano-pore fully filled with rod-like structure released by STM tip during scanning.

References:

[1] Grill, L.; Dyer, M.; Lafferentz, L.; Persson, M. V.; Hecht, S. Nat. Nanotech. 2007, 2, 687

[2] Geagea, E.; Jannoutot, J.; Feron, M.; Palmino, F.; Rochefort, A.; Thomas, C. M.; Chérioux, F. Nanoscale 2021, 13, 349

On-surface photoswitch from different AZO and DAE derivatives studied by scanning tunneling microscope

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Abstract:

Scanning tunneling microscope (STM) is a powerful technique to investigate topographic as well as electronic properties on functional organic molecules down to sub-molecular or atomic scale.[1] We have recently designed and studied ditopic ligands consisting of bipyridine (bpy) terminal groups linked through photochromic central moieties including azobenzene (AZO) or diarylethene (DAE). These molecules exhibit multi-switchable properties by different triggers such as protonation and light illumination.[2,3] Bpy-AZO-bpy and bpy-DAE-bpy molecules have been allowed to first self-organize on surface then have been photo-switched in situ. The different conformers or configurations from both systems, before and after switching, were evidenced by STM at a sub-molecular level at the solid/liquid interface.

The bpy-AZO-bpy molecules were first self-assembled with the AZO center in their flat TRANS confirmation (Figure a).[4] The orientation of the two bipyridine terminals can be modified by protonation, where "U" shape cis conformers are transformed into the "S" shape trans conformers. After UV irradiation, individual AZO units switch out of plane to their CIS conformation and are observed by STM as shown in Figure b.

The DAE photochromic center, from bpy-DAE-bpy molecule, can switch reversibly between its open- (OF) and closed forms (CF) upon visible and UV light irradiation, respectively.[5] The CF molecules show two kinds of density of states (DOS) patterns, (Figure 1c and d) representing the HOMO and LUMO, respectively. Reversible CF/OF photo-switches are evidenced on the LUMO images at a sub-molecular level. The observed images are attributed to a combined electronic DOS as well as topographic contrasts. Density function theory calculation provides a theoretical comprehension to the observed HOMO/LUMO images and the DAE switches. (Figure 2c and d). As an exciting result, the bpy-DAE-bpy molecules show a clear cooperative photo-switch.

These observations demonstrate on surface multi-functional switches at a sub-molecular level.

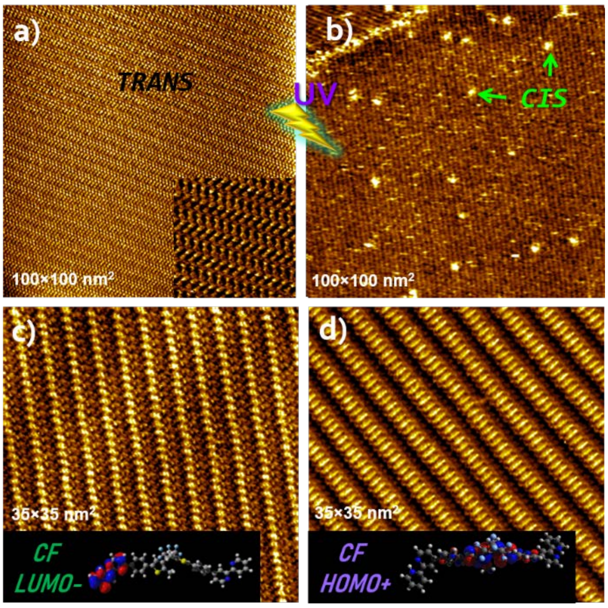

Figure 1 – STM images showing the self-organizations from bpy-AZO-bpy and bpy-DAE-bpy, respectively.

References:

[1] X. Sun*, X. Yao, G. Trippé-Allard, J. C. Lacroix*, *J. Phys. Chem. C* 2021, 125, 1, 957–963.
[2] X. Sun*, F. Lafolet*, G. Lemercier, F. Maurel, J. C. Lacroix, *J. Phys. Chem. C* 2017, 121, 20925–20930.
[3] X. Sun*, X. L. Yao, D. Frath, F. Lafolet, G. Lemercier, J. C. Lacroix*, *J. Phys. Chem. Lett.* 2019, 10, 15, 4164
[4] I. Hnid, X. Sun*, D. Frath, F. Lafolet*, J. C. Lacroix. *Nanoscale* 2019,11, 23042-23048.
[5] I. Hnid, **L. Guan**, E. Chatir, S. Cobo, F. Lafolet, F. Maurel, J. C. Lacroix*, X. Sun*. Topographic Contrasts on Cooperatively Switched Diarylethene-Bridged Ditopic ligand, *Submitted*

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

Towards tunable single molecule photon sources

Vibhuti Rai,[a] Lukas Gerhard,[a] Nico Balzer,[b] Michal Valášek,[b] Marcel Mayor,[b,c] Wulf Wulfhekel[a]

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Abstract:

Race to miniaturize light emitting diodes has led to develop interesting molecular designs capable of converting an electric current into light when connected to metallic leads. This imposes conflicting demands for the molecule-electrode coupling. To conduct, the molecular orbitals need to hybridize with the electrodes. To emit light, they need to be decoupled from the electrodes to prevent fluorescence quenching. Typically, this can be achieved by so called self-decoupled molecules that consist of a chromophore linked to anchoring groups. However, these designs are complex in nature and often the molecules either lack the needed electronic decoupling or they lack reproducibility of the light emission spectrum. Here we study the light emitting molecules in a low temperature ($\sim 4.4\ \mathrm{K}$), ultra-high vacuum scanning tunnelling microscope (STM)[1]. In this STM geometry, novel design naphthalene diimide (NDI) chromophore is linked to a gold substrate via a molecular tripod and via the vacuum barrier to the silver coated tip. This allowed us to control the fluorescence quenching by varying the vacuum barrier. The proposed tripodal anchoring group provides sufficient electronic decoupling to the light emitting chromophores, and in turn, a high quantum yield of photons/electron is observed. These molecules also allow us to probe intriguing phenomena like over-bias emission[2], and hot electroluminescence[2]. The novelty of this approach lies in the fact that this platform can be used to mount different chromophores to achieve tunable single molecule photon sources.

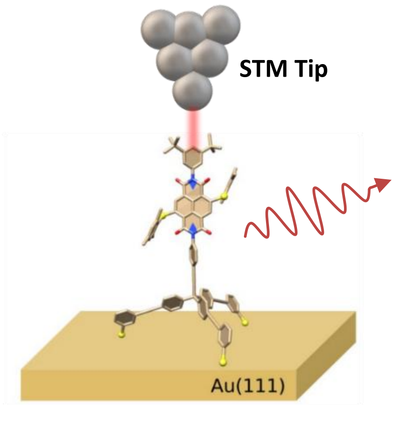

Figure : Adsorption geometry of the NDI complex on Au(111) in the STM junction.

References:

[1] K. Edelmann, L. Gerhard, M. Winkler, L. Wilmes, V. Rai, M. Schumann, C. Kern, M. Meyer, M. Wegener, and W. Wulfhekel, Rev. Sci. Instrum. **89**, (2018).

[2] Z.C. Dong, X.L. Zhang, H.Y. Gao, Y. Luo, C. Zhang, L.G. Chen, R. Zhang, X. Tao, Y. Zhang, J.L. Yang, and others, Nat. Photonics **4**, 50 (2010).

A single-molecule electronic transport survey of nanowires based on curcuminoids

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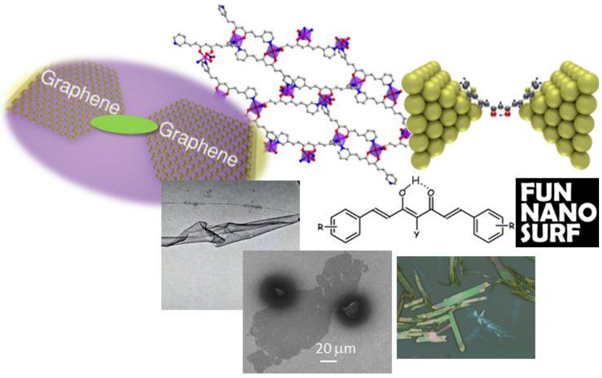
Abstract:

During the last years, my group FunNanoSurf has designed a number of curcuminoids (CCMoids) and studied them in fields related to Nanoscience and Nanotechnology aside from biomedicine.[1]

Here, I would like to emphasize our work with CCMoids in the field of Molecular Electronics, regarding single-molecule transport studies by the use of (i) break junction (BJ)[2] and (ii) mechanically controllable break junction (MCBJ)[3] techniques.



The combination of these well-developed approaches and the thorough design of the molecular units, including anchoring groups and their coordination to metal/metalloid centres, has promoted a detailed knowledge of the conductance properties of CCMoids at the single molecule level, expandable to additional families conjugated molecules.[1-3]

In addition, I will introduce our latest results in the creation of CCMoid-based extended systems (1D-3D) for electronic purposes.

References:

[1] (a) L. Rodríguez-Cid *et al.* Dalton Transactions, **2021**, 50, 7056 (b) L. Rodríguez-Cid *et al.* Cryst. Growth Des., **2020**, 20, 6555.(c) E. Castro *et al.* RSC Adv., **2018**, 8, 73, 41692. (d) R. Díaz-Torres *et al.* Chem. Sci., **2016**, 7, 2793.

[2] (a) E. Burzuri *et al.* ACS Nano, **2016**, 10 (2), 2521. (b) F. Prins *et al.* Nano Letters, **2011**, 11, 4607.

[3] (a) D. Dulić *et al.* J. Phys. Chem. C, **2020**, 124, 2698−2704 (b) I. Olavarria-Contreras *et al.* Chem. Sci., **2018**, 9, 34, 6988. (c) A. Etcheverry-Berrios *et al.* Chem. Eur. J. **2016**, 22, 12808.

Coupling plasmonic trapping and single-molecule junctions

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Abstract:

Molecular electronics (ME) is largely based on the understanding of the properties of single molecules (SM) to enable their detailed characterization. Such knowledge is aimed to define molecular properties in future implementation on molecular-based devices. Nowadays, the detection of individual molecules trapped between two electrodes[1] is a reality, and different approaches have been developed for high-precision SM trapping in fixed size nanogaps.[2] They permit from electrical characterisation of individual molecules to molecular sensing, recognition, or SM reactions.[2,3] These trapping approaches are based on the detection of SM events with lifetimes that last for a characteristic time rather short - in the order of a fraction of milliseconds - due to thermally activated junction breaking. Hence, elaborated junction characterisation is hindered over longer timescales. The detection of short junction lifetimes limits any fundamental study and therefore, immobilising molecules for prolonged timescales has remained one of ME's central challenges.

In the first block, we will present our recently reported plasmon-supported break-junction technique (PBJ)[4] based on scanning tunnelling microscopes working with the break-junction mode (STM-BJ).[1] Our PBJ technique significantly increases the lifetime of SM junctions preserving the target molecule's native structure and contact geometry. In PBJ, the exerted optical (stabilising) force of the nearfield gradient is exploited to increase the trapped molecule junction stability, without the need for chemical modification of the target molecule and/or electrode. The optically induced mechanical stabilization of the trapped molecule is suitable at low and moderate far-field power densities and successfully overcomes the native stochastic disconnection of the junction, imposing a deterministic lifetime.

In the second block, we will explain how the steering of two physical features can extend the effectiveness of the nearfield trapping[5] in the PBJ: (i) the target molecule's optical resonance and (ii) the localised surface plasmon resonance (LSPR) energy of the nanogap. Our target molecule, the metalloprotein Azurin (Azu), has a Cu(II) metal centre that when oxidised possesses an intense absorption ligand-to-metal charge transfer band, resonant to the employer laser frequency to excite the Au plasmon. Thanks to the electrochemical (EC) gating capabilities of our approach, we can tune the resonant excitation conditions of the trapped Azu via modifying its Cu centre's redox state. Consequently, when Azu is oxidised presents resonant conditions, and therefore, its electric polarizability is enhanced. Since the emerging gradient force of the nearfield is proportional to the polarizability, the higher is the polarizability, the larger is the efficiency of the molecular trapping. In parallel, the tuning of the nanogap's LSPR energy can be also used to enhance the molecular trapping. LSPR energy profile depends on the applied electrode potential determined by the Fermi level displacement which we control via the EC gate. The LSPR energy profile is correlated with the wavelength-dependent electric field enhancement that controls the nearfield exerted force, and thus tunes the optical trapping efficiency and junction lifetime. Our results demonstrate that the optical trapping of individual molecules is suitable, and hence it enhances the molecular sensing and recognition.

References:

1 B. Xu and N. J. **Tao**, ***Science***, 2003, 301, 1221.
2 A. C. **Aragonès**, et al ***Nature***, 2016, 531, 88.
3 A. C. **Aragonès** et al, **J. Am. Chem. Soc**. 2017, 139, 5768.
4 A. C. **Aragonès** and K. F. Domke, ***Cell Rep. Phys. Sci.***, 2021, 100389.
5 A. C. **Aragonès** and K. F. Domke, ***J. Mater. Chem. C*** 2021, DOI: 10.1039/D1TC01535D.

Long-lived charged states in porphyrin nanoribbons

Edmund Leary,[a,b,c] Georg Kastlunger,[d,e] Bart Limburg,[f] Laura Rincón-García,[g] Juan Hurtado-Gallego,[g] M. Teresa González,[a] Gabino Rubio Bollinger,[g,h] Nicolás Agrait,[a,g,h] Simon J. Higgins,[b] Harry L. Anderson,[f] Robert Stadler[i] and Richard J. Nichols.[b,c]

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Abstract:

We will demonstrate that sub-5 nm porphyrin nanoribbons[1] can be charged inside two-terminal single molecule junctions in which the charged state can persist for many seconds under ambient conditions.[2] This phenomenon is possible due to the presence of a localized molecular eigenstate close to the Fermi edge of the electrodes which can be accessed by applying a moderately high bias voltage of about 1.0 V. Upon charging, the low-bias molecular conductance is boosted by approximately two orders of magnitude which gives rise to a hysteretic *I-V* response. This opens the door to the tantalizing possibility that these long-lived charged states may lead to memristor architectures or redox-based molecular memories in future two-terminal devices. The ambient operation highlights that special environments, low temperatures or ultra-high vacuum conditions are not prerequisites for stable charged molecular junctions.

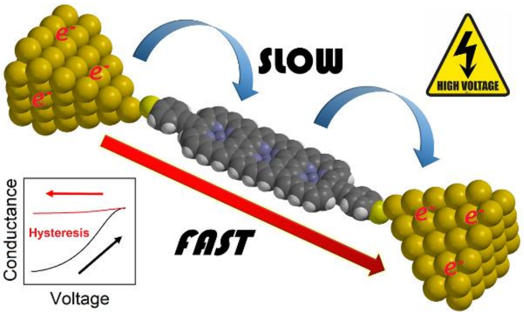

Figure 1. Schematic demonstrating the two channel mechanism of charge transport in porphyrin nanoribbons.

References:

(1) - , N.; Higgins, S. J.; Lambert, C. J.; Anderson, H. L.; Nichols, R. J. Bias-Driven Conductance Increase with Length in Porphyrin Tapes. *J. Am. Chem. Soc.* **2018**, *140* (40), 12877–12883.

(2) Leary, E.; Kastlunger, G.; Limburg, B.; Rincón-García, L.; Hurtado-Gallego, J.; González, M. T.; Bollinger, G. R.; Agrait, N.; Higgins, S. J.; Anderson, H. L.; Stadler, R.; Nichols, R. J. Long-Lived Charged States of Single Porphyrin-Tape Junctions under Ambient Conditions. *Nanoscale Horiz* **2021**, *6* (1), 49–58.

Invited Speaker

Quantum Interference in Single-Molecule Circuits

Latha Venkataraman

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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.

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Electronic Motor Based on Single Tripodal Chiral Molecule

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Abstract:

We present our results concerning a single molecular motor driven by the current in an STM. The investigated molecules are tailor-made in the group of Prof. Mayor. The three anchoring groups fix the molecules to the Au(111) surface they are deposited onto (see Fig.1). The functional group is supposed to perform a rotation in a preferred direction with respect to the anchoring groups. The proposed mechanism to drive the directed motion is based on the chiral-induced spin selectivity (CISS) effect. This effect causes the electron spin of an injected current to be polarized after passing through a chiral electric field [1]. This spin polarization exerts a torque on the functional group via spin-orbit coupling. Therefore, the functional group is chosen to be chiral. By comparison with previously studied, similar molecules, it can be concluded that the molecules adsorb with the anchoring groups on the Au(111) surface. This leaves the chiral group roughly perpendicular to the surface and free to rotate.

Indeed, when positioning the tip above the molecule, abrupt changes in the tunneling current can be observed. Tip positions can be found where the current switches between three distinguishable current levels without moving the tip (see Fig.2). These current levels are interpreted as metastable rotational states (called A,B and C) of the molecule. That way, two directions A->B->C and C->B->A can be defined. A binomial test is used to determine whether the surplus of rotational switches in one direction compared to the other is statistically significant. Our measurements show clearly, that the observed directional rotation is statistically significant. The highest ratio observed in the switching events in the different directions is 489 to 36.

In addition, bias voltage dependent measurements were performed. Here, we see a clear trend that the number of switching events increases monotonically with increasing bias. However, the asymmetry in the switching events, which is a measure for the drive of the directed motion, exhibits non-monotonic behavior.

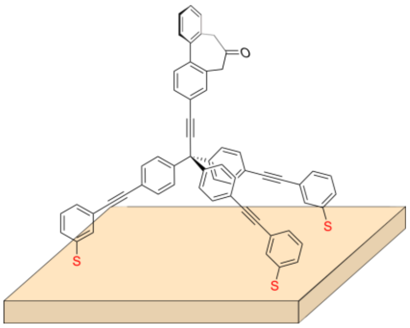

Fig.1: Molecular Motor Molecule

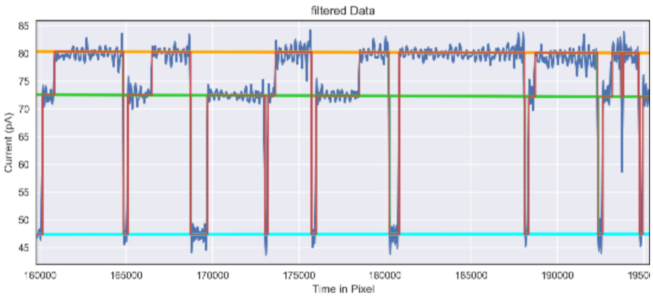

Fig.2: Example of measured metastable current levels

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[1] Naaman, R.; Waldeck, H.; Chiral-Induced Spin Selectivity Effect, J. Phys. Chem. Lett. 2012, 3, 16, 2178 - 2187

Single Molecule Junctions from metal-complex molecules: Long range charge transport, stability and I/V characteristics

Xilei Yao,[a] Maxime Vonesch, [b] Frédéric Lafolet,[a] Jean Weiss, [b] **Xiaonan Sun, [a*]** and Jean-Christophe Lacroix[a*]

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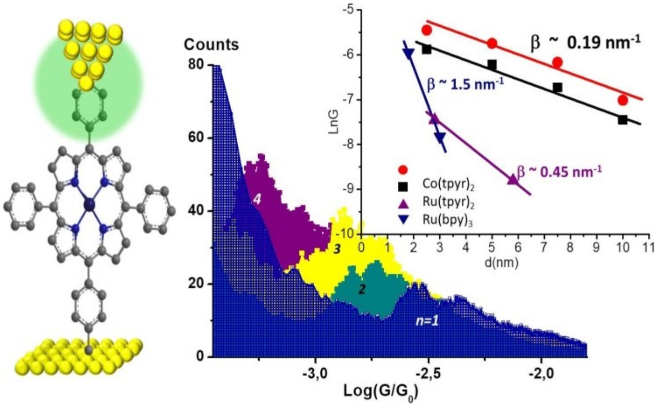
Abstract:

The research of single molecule junction (SMJ) aims to miniaturize the molecular electronics in size and to optimize the charge transports in efficiency. A SMJ is formed when a single molecule is connected between two conducting electrodes. We have recently studied SMJs, based on two types of organometallic oligomers. They are deposited as ultrathin layers on an ultraflat gold bottom electrode and are contacted by an STM tip used in various modes (STM-break junction or I(t) mode).

The first systems are based on Au-[metal-$(tpy)_2$]n-Au (n = 1–4). Highly efficient long range transport is observed from Au-$[Co(tpy)_2]_n$-Au SMJs where the conductance (~10^{-3} G_0) shows very weak length dependence. An extremely low attenuation factor (β~0.19 nm^{-1}) is obtained which indicates that resonant charge transport is the main transport mechanism. By varying the SMJ metal center from Co to Ru, the conductance decreases by 1 order of magnitude. In Au-$[Ru(tpy)_2]_n$-Au and Au-$[Ru(bpy)_3]_n$-Au SMJs, a charge transport transition from direct tunneling to hopping is evidenced from the length-dependent β-plot in the right figure. Three different transports mechanisms are observed with clear molecular signature. (1)



In a second system, Au-[metal-porphyrine]$_n$-Au SMJ is studied on both their transport properties and their stability by recording the SMJ life time, namely the G(t) measurements. Au-[NH_2-CoTPP]n-Au SMJs show random telegraph G(t) signals first then stabilize with a surprisingly long lifetime around 10s.(2) By adding an extra NH_2 anchoring group, Au-[NH_2-CoTPP-NH_2]n-Au SMJs are recorded to stabilize with a life time as long as 1 min. Thanks to the high stability, intensive I(V) measurements at a single molecule level are easily feasible. The I/V characteristic from different SMJs indicates that, the applied bias voltage decreases the attenuation factor and drives the device toward resonant tunneling. (3)

We have therefore obtained SMJs with unprecedented stability and studied their transport properties using three complementary characterizations: the STM-bj G(d) histogram, the stability from G (t) and the voltage dependent conductance G(V) measurements. The observed unprecedented stability is likely due to a combined contribution: the diazonium grafting covalently immobilizes molecules and impedes molecule movements; the anchoring groups optimize the top molecule-tip contact.

References:

(1) X. Yao, X. Sun*, F. Lafolet, J. C. Lacroix*, *Nano Lett*. **2020**, 20, 9, 6899–6907.
(2) X. Yao, M. Vonesch, M. Combes, J. Weiss, X. Sun*, J. C. Lacroix*, *Nano Lett.* **2021**, 21, 15, 6540–6548.
(3) X. Yao, M. Vonesch, J. Weiss, X. Sun*, J. C. Lacroix*, *to be submitted.*

Electron-phonon interactions in weakly coupled single-molecule junctions

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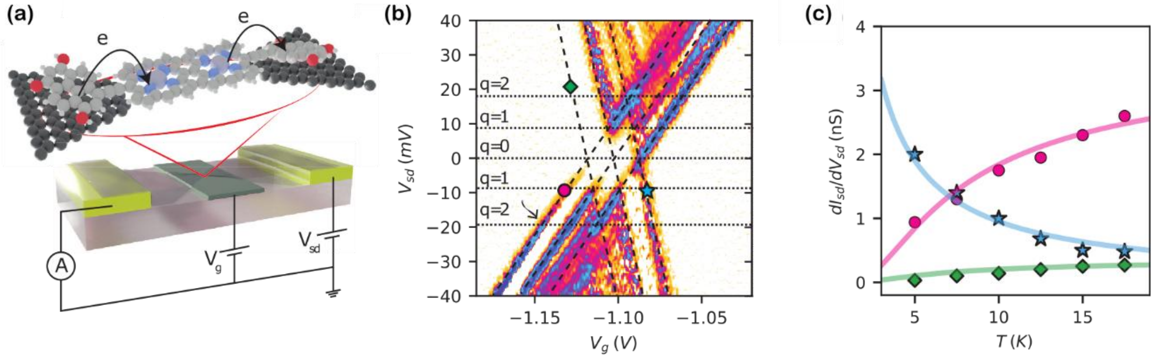
Abstract:

Off-resonant charge transport through molecular junctions has been extensively studied since the advent of single-molecule electronics and is now well understood within the framework of the non-interacting Landauer approach. Conversely, gaining a qualitative and quantitative understanding of the resonant transport regime has proven more elusive. Here, using a three-terminal device architecture,[1] resonant charge transport through weakly coupled graphene-based single-molecule junctions will be described.[2] The inadequacies of non-interacting Landauer theory will be demonstrated, and through a combination of temperature- and gate-voltage- dependent measurements of conductance the interplay between Marcus Theory and quantum descriptions of electron-phonon coupling will be unravelled. Furthermore, the observance of vibrational sidebands[3] in the Coulomb-blocked regions of charge transport provides experimental evidence of non-equilibrium vibrational dynamics in single-molecule junctions and allows vibrational relaxation times to be extracted that are orders of magnitude slower than expected from solution-phase electronic spectroscopy.[4]



(a) Architecture of three-terminal graphene–based single-molecule transistors. (b) Conductance map of resonant transport, displaying vibrational side-bands in the Coulomb-blocked regions. (c) Bosonic temperature dependence of vibrational signatures.

References:

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[4] Thomas et al. in preparation (2021)

Highly efficient photoswitch in diarylethene-based single- and bi-layer molecular junctions

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Abstract: Photochromic molecules, that is, molecules with two different forms (open/non conjugated and closed/conjugated) which can be interconverted by light irradiation, have been proposed as building blocks for photoresistive switches in molecular electronics[1]. Diarylethenes (DAE) are among the molecules that have been extensively investigated due to their excellent properties such as the high reversibility, thermal stability and fatigue resistance of both forms. Most studies, investigating the transport characteristics of photochromic molecules, are devoted to monolayers or single-molecule-based Molecular Junctions (SMJs) where the dominant transport mechanism is direct tunneling. Hopping transport, whichhas a stronger molecular signature, has remained almost unexplored. Herein we present the electrical characterization of photoswitchable MJs using molecular layers of diarylethene oligomers (oligo(DAE)) for tunneling and hopping transport regimes.

First, we prepared single-layers of the oligo(DAE) deposited by electrochemical reduction on gold electrodes with several thicknesses. The layers were fully characterized using electrochemistry, XPS, and AFM. The electrical characterization of closed and open forms of oligo(DAE) were investigated by C-AFM and will be presented for two different layer thicknesses fixed at 2-3 nm and 8-9 nm, i.e. below and above the direct tunneling limit. It was observed that both layers switch between high and low conductance modes (“ON” and “OFF” states corresponding to “closed” and “open” forms of the oligo(DAE), respectively) when irradiated by UV and visible light, respectively. ON/OFF ratios of 2-3 (Fig.1.A) and 200-400 (Fig.1B) were obtained for 3 nm- and 9 nm-thick DAE MJs, respectively[2].

Next, we prepared, using a bi-layer system, 9 nm-thick MJs, i.e. in the hopping transport regime. The first layer (5 nm) is based on bisthienylbenzene oligomers, (BTB). The second layer (4 nm) is based on the oligo(DAE). The impact of this first layer on the switchable properties of the system and on the electronic behavior and on the photoresponse of the 9 nm-thick DAE-based MJs will be presented, with focus on its influence on the ON / OFF ratios (Fig.1C). Unprecedented ON/OFF ratio of 10000 at 1V were observed. [3]

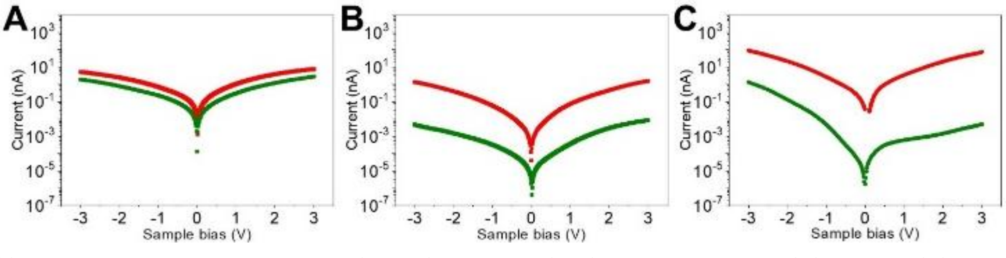

Fig.1. Log(I) versus V characteristics before (green) and after (red) UV irradiation of (A) DAE$_{3nm}$, (B) DAE$_{9nm}$, and (C) DAE$_{4nm}$/BTB$_{5nm}$ junctions measured by C-AFM.

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1. Huang X, Li T. Recent progress in the development of molecular-scale electronics based on photoswitchable molecules. *J Mater Chem C*. 2020;8(3):821-848.
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3. Hnid I, Liu M, Frath D, Bellynck S, Lafolet F, Sun X. Unprecedented ON/OFF Ratios in Photoactive Diarylethene-Bisthienylbenzene Molecular Junctions. *Nano Lett*. doi:10.1021/acs.nanolett.1c01983

Non-volatile Memory in Large-area Junctions Comprising Self-assembled Fused Porphyrins

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[b]Department of Chemistry, Chemistry Research Laboratory, University of Oxford, Oxford OX1 3TA, United Kingdom
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Abstract:

The invention of next-generation computing primitives that keep up with the exponential increase in data storage and computing demand has become one of the greatest challenges in materials science and IT engineering.[1] Human brains outperform the best computers in the world in many complex problems, such as decision-making. This inspiration has led to the creation of inorganic/organic electrical materials and device architectures for neuromorphic computing to emulate the functions of human brains. However, their energy-efficiency, performance under working conditions and reproducibility for scalable production remain as the major bottlenecks.

Molecular self-assemblies, the ordered structures formed by spontaneous covalent/non-covalent interactions between molecules and substrates, have the solution to those challenges. When integrated into electronic devices, they display quatum-transport properties which can be fine-tuned by changes at atomic scale.[2] Pioneering work has demonstrated that charge-transport through molecular self-assemblies can be modulated by electric fields and ionic/molecular recognition at low power cost;[3-6] however, molecular self-assemblies that are responsive to multiple stimuli and operate in a stateless fashion, which is one of the key features of human brains, are yet to be developed.

During this lecture, we will present our recent progress in synthesizing non-volatile memory from large-area junctions comprising self-assembled monolayers of redox-active fused porphyrins.[7] These self-assembled monolayers exhibit reversible, multi-state switching in electrical conductance which is driven by (partial) oxidation/reduction under electric fields in "WRITE-READ-ERASE" operations. An investigation into the charge-transport mechanism reveals a complex picture in which resonant tunneling and thermally activated charge-transfer intertwine. The unique system is multi-responsive, enabling modulation of its conductance states from electrical bias and temperature, which can be trained to recognize stimulations retrospectively.

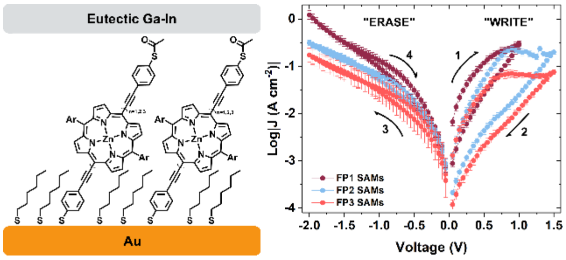

Figure 1. The schematic of the large-area junction comprising self-assembled fused porphyrins (FPn) and eutectic Ga-In top electrode (left), and the J-V curves during "WRITE-ERASE" operations (right).

References:

[1] J.D. Kendall, et al., Appl. Phys. Rev. 2020, 7, 011305; [2] M. Carlotti, et al., Nat. Commun 2016, 7, 13904; [3] Y. Ai, et al., Nano Lett. 2018, 18, 7552-7559; [4] X. Qiu, et al., Nat. Mater. 2020, 19, 330-337; [5] Y. Han, et al., Nat. Mater. 2020, 19, 843-848; [6] X. Qiu, et al., Adv. Mater. 2020, 2006109. [7] X. Qiu, et al., Manuscript in preparation 2021.

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

Invited Speaker

Towards functional high-yield molecular electronic devices

Takhee Lee

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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].

References:

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Information encoding and energy harvesting using the ferromagnetic metal /molecule interface in quantum spintronic vertical nanodevices

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Abstract:

Molecular spintronics is emerging as a vibrant field that utilizes the properties of magnetic molecules toward additional device functionalities that can exploit quantum physics. One spectacular property is the high spin polarization of the ferromagnetic metal/molecule interface, measured at 300K using spectroscopy [1] and magnetotransport [2] experiments.

The magnetism of this so-called spinterface [3] can be controlled using an underlying ferroelectric [4], and can in principle be combined with a molecular function (e.g. spin crossover) by inserting a noble metal spacer layer [5,6] (see Weber talk). The spinterface formation entails changes to the magnetic properties of the interface constituents, from magnetic hardening of the metal [7] to the magnetic stabilization of otherwise paramagnetic molecular spin chains borne by phthalocyanine (Pc) molecules [8]. These effects enable the encoding of information into the quantum state of a molecular spin chain within vertical solid-state nanojunctions[9]. This constitutes a promising applicative implementation of first results on STM-assembled and laterally-assembled model junctions [10].

The interaction between the spinterface and a molecular spin chain also lays the groundwork for a molecular implementation [11] of our recent proposal [2] (www.spinengine.tech) to harvest the energy of thermal fluctuations on paramagnetic centers using spintronics and quantum thermodynamics. The observed output power, and industrial maturity of spintronics, suggest[2] that this technology could be very competitive relative to the harvesting of other natural (e.g. solar cells) and artificial (e.g. wifi/GSM).

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[11] B. Chowrira, L. Kandpal et al, arXiv : 2009.10413

Diarylethene self-assembled monolayers on cobalt with high conductance switching ratio for spintronics

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The use of photochromic and electrochromic active molecules in molecular junctions allows modulating the electron transport response of these molecular junctions using light or electric field. When these molecules are used with ferromagnetic (FM) electrodes, the spin-polarized electron transport through the FM/molecules/FM junctions will depend on the conformation of the molecules and the molecule/electrode atomic contact geometry, as evaluated from theoretical studies.[1-3] We have recently reported the optically induced conductance switching at the nanoscale (conductive-AFM) of diarylethene derivatives self-assembled monolayers (SAMs) on $La_{0.7}Sr_{0.3}MnO_3$ electrodes,[4] and observed a weak conductance switching of the diarylethene molecular junctions (closed isomer/open isomer conductance ratios $R_{c/o} < 8$) and conductance ratio (cis/trans isomers) of about 20 for azobenzene derivatives on Co.[5] Here, we report an unprecedented $R_{c/o} \approx 400$ for diarylethene SAMs on Co (against ≈ 50 for the same SAMs on Au). The molecules (DAE1 and DEA2, see Figure) were designed and synthesized diarylethene for large conductance switching ratios. The electron transport properties of SAMs on Au and Co were measured by conductive atomic force microscopy (C-AFM in air and UHV, respectively) coupled with first principle calculations (Non-Equilibrium Green's Functions combined with Density Functional Theory, NEGF/DFT). The experiments and calculations agree on the following trends: (i) Both molecules show a higher $R_{C/O}$ on Co than Au; (ii) With both metals, the $R_{c/o}$ for DAE2 is higher than for DAE1. We conclude that these DAE molecular junctions on Co are prone to magnetoresistance measurements at the nanoscale (in progress).

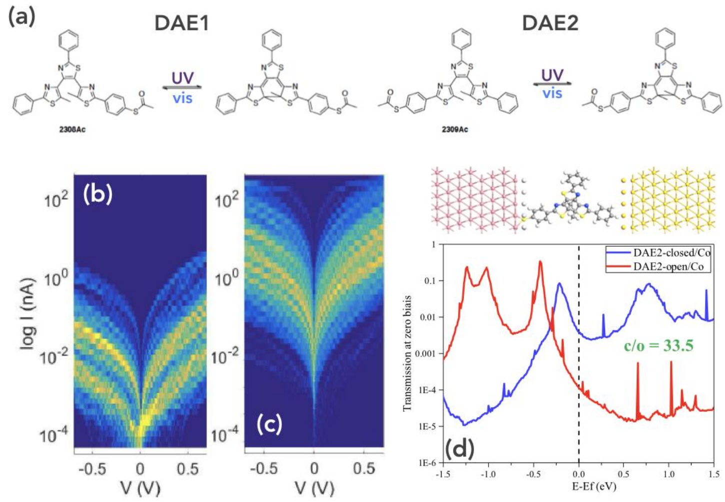

Figure. Scheme of DAE1 and DAE2 (a), 2D histograms of the CAFM tip/DEA2/Co junctions in the open (b) and closed (c) forms, and the calculated transmission coefficients (d).

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

Spin-dependent transport through photoswitchable Self Assembled Monolayers

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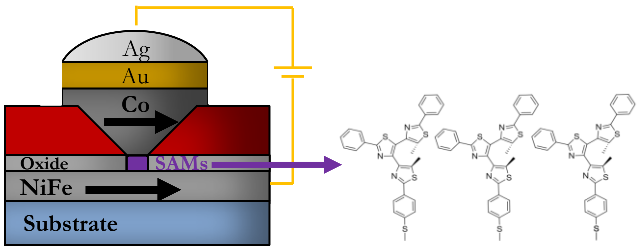
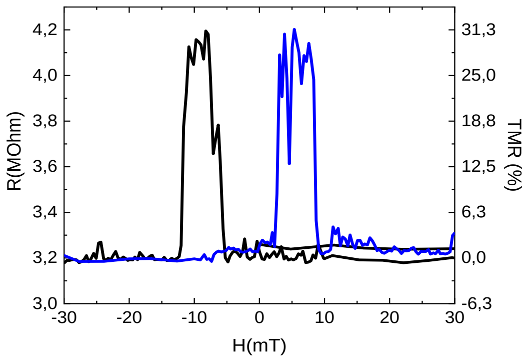
Abstract:

Magnetic tunnel junctions (MTJs) are known to be one of the main building blocks of spintronics. In these devices, the integration of molecular layers as tunnel barrier is envisioned as an opportunity to allow the engineering of spintronics at the molecular scale. Actually, thanks to the spin-dependent hybridization at ferromagnet/molecule interfaces, it was shown that one could now expect to tailor spin polarization and thus tunnel magnetoresistance (TMR) with molecules (a.k.a. spinterface) [1]. In this direction, among the wealth of molecular systems, self-assembled monolayers (SAMs) appear as one of the most promising tool to tailor the MTJs tunnel barrier. Indeed, as shown in molecular electronics, their properties could be finely tuned at the molecular level. Pioneer experiments have shown that "passive" molecules such as alkane chain could be integrated into MTJs [2].

In this talk we will present the first work integrating "active" diarylethene molecules in NiFe/diarylethene/Co MTJs molecular MTJs. As the electron delocalization, energy gap and coupling strength to the electrodes depend on the molecule state, the tunnel resistance and tunnel magnetoresistance (TMR) is expected to be tuned upon switching. We will first present our optimized fabrication process that enables to work with ferromagnets in solution and fabricate working molecular MTJs. We will then discuss the electronic and TMR properties obtained in both open and closed forms of the diarylethene molecules. Finally, we will show that this work demonstrates that switchable "active" molecules can be successfully integrated into MTJs towards multifunctional molecular spintronic devices electrically and/or optically controllable.





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Invited Speaker

Ionic Gating of 2D Semiconductors

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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 μF/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.

Borophenes made easy: Distinct polymorphs and heterostructures

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[2] *Département de Chimie, Ecole Normale Supérieure, France*
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Abstract:

Surface-supported two-dimensional (2D) materials keep attracting considerable interest. For example, borophene, a synthetic, boron-based 2D material, offers intriguing anisotropic electronic and mechanical properties [1,2]. Here, we present a versatile chemical vapor deposition (CVD) approach to grow atomically-thin 2D polymorphs of borophene by using diborane. This precursor originates from byproducts of commercial borazine, a popular material for growth of hexagonal boron nitride (*h*BN). Specifically, borophene polymorphs with large single-crystalline domains are synthesized on Cu(111) and Ir(111) supports. Additionally, atomically-precise lateral interfaces or vertical van der Waals heterostructures combining borophene and *h*BN can be achieved by sequentially dosing different precursors from the same supply (Fig. 1). Thereby, borophene is protected from immediate oxidation by encapsulation with a single *h*BN overlayer. The borophene polymorphs and interfaces with *h*BN are comprehensively characterized by low-temperature scanning tunneling microscopy and spectroscopy, x-ray photoelectron spectroscopy, low energy electron diffraction and complementary density functional theory modeling [3]. The ability to synthesize high-quality borophenes by a straight-forward, scalable CVD approach opens up opportunities for the study of their fundamental properties and for device incorporation.

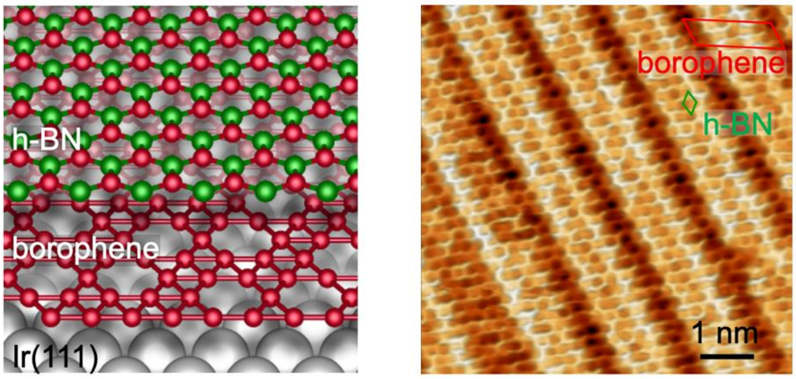

Fig. 1. Scheme (left panel) and atomically-resolved STM image (right panel) of a vertical heterostructure with h-BN covering borophene on Ir(111).

References:

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ElecMol
10th International Conference on Molecular Electronics
ElecMol20
14-17 December 2020
ENS de Lyon

Spin crossover/graphene heterostructure based switchable optoelectronic devices

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Abstract:

Spin crossover (SCO) molecular materials exhibit a change of magnetic state that can be triggered by several external stimuli, in particular temperature, pressure, electric field and light irradiation. Despite their important potential, their use in multi-functional devices is hampered by several technological locks: (i) optoelectronic devices remain scarce because of complex intricate phenomena into the SCO channel, (ii) the low intrinsic conductivity of SCO material prevent their use for several sensing applications, (iii) optoelectronic switch based on SCO phenomena and operating at room temperature is very difficult to achieve. Today, I will present some of our recent achievements and on-going works illustrating the possibilities offered by ***SCO-2D materials heterostructures*** for optoelectronic applications, and how they can unlock these challenges.

First, magneto-opto-electronic properties are shown for a hybrid device constructed from a spin crossover (SCO) thin film of the $Fe[HB(3,5\text{-}(Me)_2Pz)_3]_2$ molecular material evaporated over a graphene sensing layer. The principle of electrical detection of the ***light-induced spin transition*** (LIESST) and reverse-LIESST effects in SCO/graphene heterostructures is demonstrated. **[1]** The switchable spin state of the molecular film is translated into a remanent change of the conductance of the graphene channel, using two distinct excitation wavelengths to write/erase the two states.

Then, I will present a hybrid device that can be switched at ***room temperature*** using light irradiation with non-volatile memory effect. The device is made of a graphene detector over which nanoparticles of the spin crossover $[Fe(Htrz)_2(trz)](PF_6)$ are deposited. For this molecular system, device operation at room temperature is realized, with multi-state stabilization obtained by varying the irradiation intensity or time. **[2]**

These results demonstrate how the electronic states of insulating molecular switches can be stored, read and manipulated by multiple-stimuli while transducing them into low impedance signal thanks to two-dimensional detectors. It reveals the full potential of mixed-dimensional heterostructures for molecular (opto)electronics and spintronics, and opens the door to the use of spin crossover materials for room temperature optoelectronic operations.

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[2] J.F. Dayen et al., *submitted* 2021**.**

Magnetic field control of the Franck-Condon coupling of few-electron quantum states[1]

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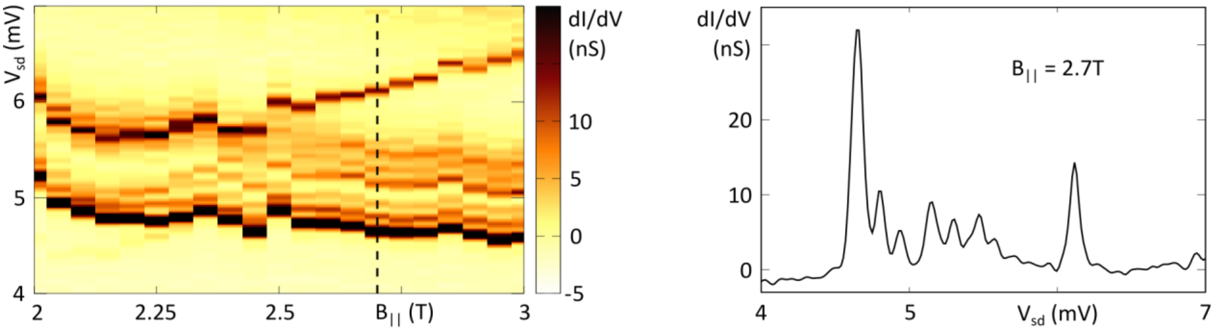
Abstract:

The longitudinal vibration of a suspended carbon nanotube has been observed many times in low temperature transport spectra via distinct harmonic Franck-Condon sidebands.[1-5] Typically, strong Franck-Condon coupling has been attributed to disorder-induced or deliberately targetted charge localization. Here, we present the observation of a strong, tunable coupling in an ultra-clean carbon nanotube with N=1 or N=2 electrons in the conduction band.

The clean transport spectrum allows a tentative identification of the electronic base quantum states according to their valley quantum number. Interestingly, the Franck-Condon coupling strength g, as extracted from our data, both depends on the magnetic field and on the precise electronic quantum states participating in transport. While spin-dependent Franck-Condon phenomena have already been observed,[6] our results clearly point towards a valley-dependent origin

As possible cause of this phenomenon, re-shaping of the electronic wavefunction envelope by the magnetic field[7-9] is discussed. A simple calculation demonstrates that variations of g as observed in the experiment can be reproduced by the theory, paving the way towards more realistic and detailed quantum-mechanical modelling.



Franck-Condon sidebands in the two-electron excitation spectrum. From Ref. 1.

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Invited Speaker

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

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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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Organic chiral radicals with SOMO-HOMO inversion: A new approach to design stable chiral open-shell materials

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Abstract: Chiral π-conjugated materials have recently emerged as a promising direction in material science due to their specific interaction with CP-light and the potential of the latter in several domains of applications such as organic light-emitting diodes (OLEDs), organic field-effect transistors (OFETs) and magnets.[1] While extensive researches have been focusing on organic closed-shell chiral dyes, a few attention has been given to their open-shell counterparts due to their low configurational stability and high chemical reactivity.[2] This presentation will illustrate our last result regarding the design of stable organic chiral mono- and diradicals based on C_2-symmetric bicarbazole derivatives.[3] Investigations of their optoelectronic properties revealed a high chemical stability for unprotected carbazole axial radical $\mathbf{1}^{\bullet+}$, in comparison to unstable helical $\mathbf{3}^{\bullet+}$ (Figure 1), owing to an uncommon SOMO-HOMO inversion and a different electronic coupling between the radical center and the electron rich unit bearing the HOMO. Such findings notably allowed us to further design and isolate chemically and configurationally stable chiral diradical $\mathbf{2}^{2\bullet2+}$, which displayed promising near-infrared chiroptical properties and nearly degenerate singlet-triplet ground states (Figure 1).

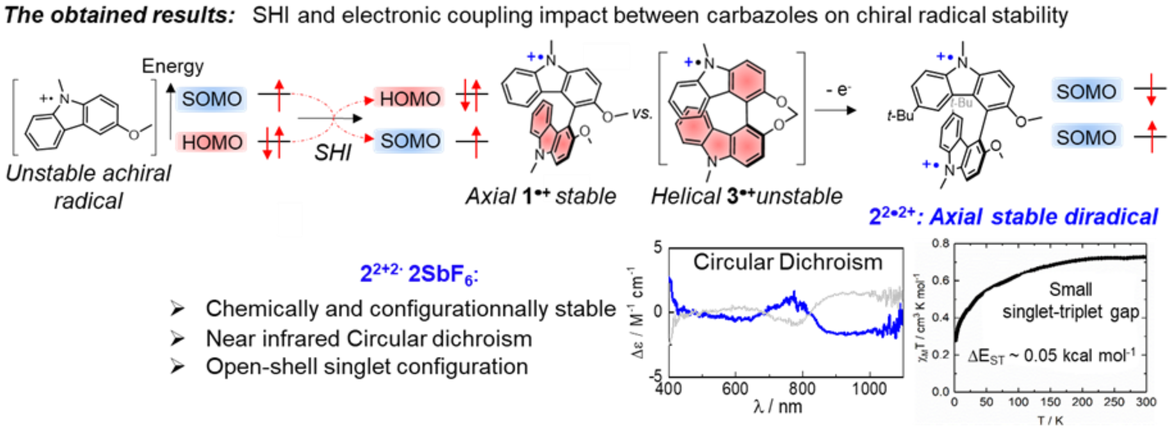

Figure 1. Chiral monoradicals showing a SOMO-HOMO inversion with colors illustrated spin distribution; plot between product of molar magnetic susceptibility (χ) and T vs T of diradical $\mathbf{2}^{2\bullet2+}$ showing curie constant (C) equal to 0.79 cm^3 K mol^{-1}, and g_{abs} of $\mathbf{2}^{2\bullet2+}$ from NIR-ECD.

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Key features for efficient long-lived room temperature persistent luminescence of organic molecular crystals

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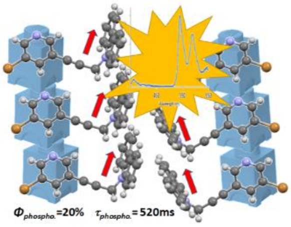
Abstract:

Room-temperature long-lived persistent luminescence from metal-free organic materials has recently attracted renewed attention from fundamental and application point of view.[1-3] This afterglow luminescence has gained increasing interest as a viable alternative to well-studied inorganic phosphorescence based on toxic, rare, and expensive elements. However, the realization of organic systems, mostly molecular crystals, with long-lived emission remains a formidable challenge, since the features of the persistent luminescence strongly depend on the electronic properties of the molecular components and on their molecular packing in the crystal.

Here, a new strategy is developed by rationally designing molecular 'phosphors' incorporating and combining for the first time a bridge for σ-conjugation between the D and A units and a structure-directing unit for H-bond-directed supramolecular self-assembly.[4] Quantum chemical calculations highlight the critical role played by the two degrees of freedom of the σ-conjugated bridge, on the chromophore optical properties. The molecular crystals exhibit room-temperature 'phosphorescence' quantum yields up to 20% and lifetimes up to 520 ms. On the other hand, the crystal structures establish the existence of an unprecedented well-organization of the emitters into two-dimensional (2D) rectangular 'columnar-like' supramolecular structure stabilized by intermolecular H-bonding. We also elucidate the underlying spin-and photo-physics of ultralong-lived light emission by demonstrating that the 'doping' by an isomer plays a crucial role.[5]



'Columnar-like' supramolecular structure stabilized by intermolecular H-bonding as structural key parameter.[4]

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

Cavity Effect in Low Volage Operating Organic Field Effect Transistors

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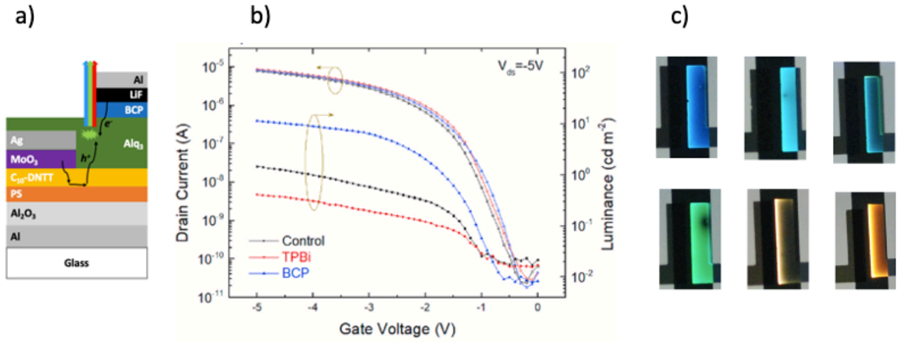
[d]Department of Chemistry, Graduate School of Science, Tohoku University, 6-3 Aoba, Aramaki, Aoba-Ku, Sendai, Japan

Abstract:

The study of organic electronics is meant to reach ways to produce electronics with alternative processes than inorganic electronics, easier to fabricate with low costs. Among many organic electronic devices, such as Organic Field Effect Transistor (OFET), Organic Light Emitting Diodes (OLED) or also Organic Photovoltaics (OPV), a particular device called "Organic Light Emitting Transistor" (OLET) is the object of recent studies. An OLET is the combination of the switching properties of an OFET with the light emitting properties of an OLED. Therefore, OLET is considered to have a great potential either for display technologies or for lasing applications.(1) Here, we present our recent study where two hole blocking molecules were integrated into Alq_3 based light emitting transistors under operating voltage as low as 5 V. The effects of hole blocking and electron injection were decoupled through the differences in the energy levels of these molecules.(2) In the follow up study, the thickness of the emissive layer was varied. By doing so, a tuning of the color was observed, going from blue to red with the exact same molecule, emitting normally in the green. A resonant cavity phenomenon was actually taking place in the structure. Optical simulations have been carried out to understand the mechanism.



a) OLET device structure in our study; b) Transfer and luminance curves of OLETs; c) Color tuning following the change in the thickness of the emissive layer

References:

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Invited Speaker

Porphyrin-Based Molecular Wires

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Email: harry.anderson@chem.ox.ac.uk

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]

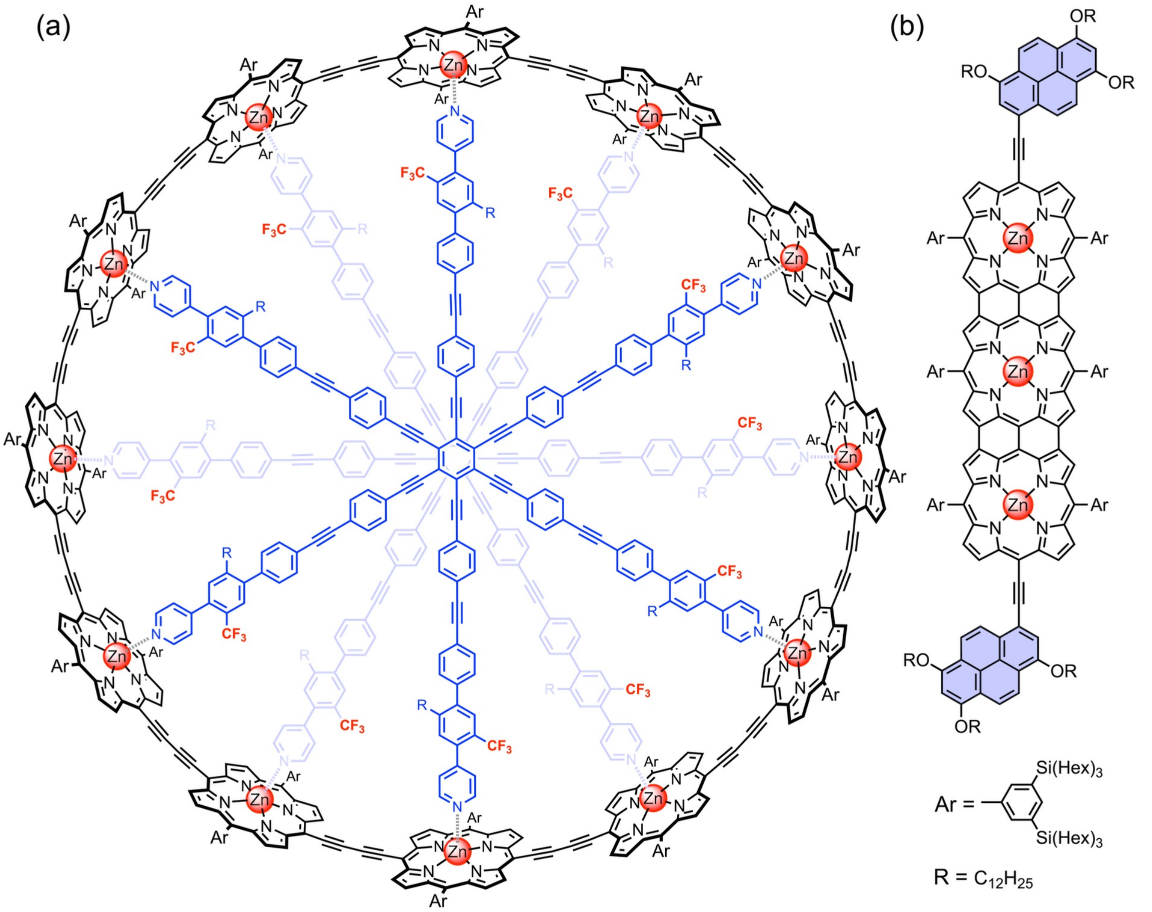

Figure 1. (a) A cyclic porphyrin dodecamer bound to two molecules of a ***T6*** *template.*[3] *(b) A fused porphyrin trimer with alkoxypyene anchor groups.*[5]

References:

[1] M. D. Peeks et al. *J. Am. Chem. Soc.* **2017**, *139*, 10463. [2] E. Leary et al. *J. Am. Chem. Soc.* **2018**, *140*, 12877. [3] M. Rickhaus et al. *Nature Chem.* **2020**, *12*, 236. [4] E. Leary et al. *Nanoscale Horiz.* **2021**, *6*, 49. [5] J. O. Thomas et al. *submitted*; https://arxiv.org/abs/2105.00487

Four modes of electrical conductivity extending over four orders of magnitude observed in extractant based microemulsions

Thomas Zemb[a], Tobias Lopian[a,b], Sandrine Dourdain[a], Jean-François Dufrêche [a]
and Werner Kunz[b]

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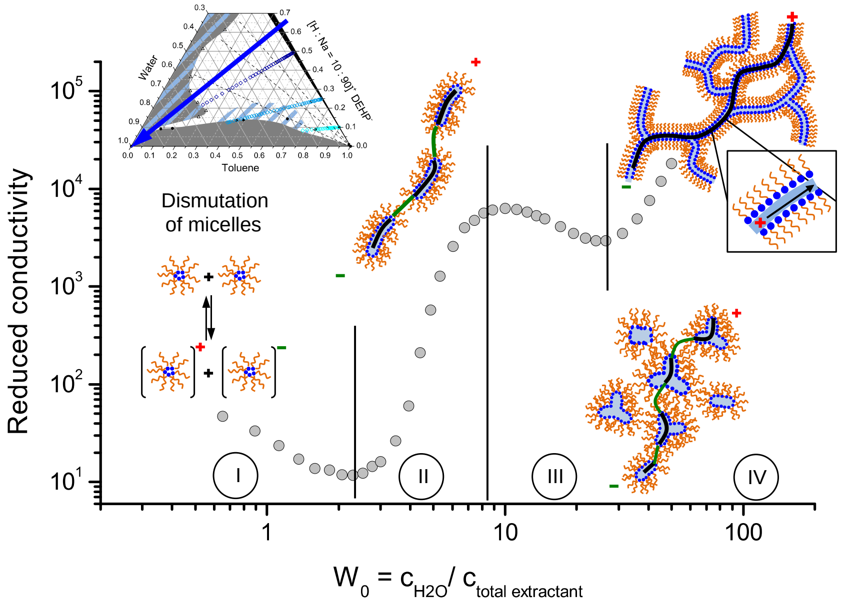
Abstract:

Reverse micelles and microemulsions are the core of all liquid-liquid extraction and recycling processes. Liquid-liquid extraction is currently the only known method to recycle magnets that are present in wind-mills. All known liquid-liquid extraction use the so-called Winsor II regime later renamed emulsification failure when a reverse micelle equilibrium is in equilibrium with excess water that contains the metallic cations that need to be selectively extracted and stripped back.

We use as model system the HDEHP an electrolytic but oil-soluble surfactant that is called “extractant” in the context of chemical engineering, for which the quaternary phase prism is available. The HDEHP/water/isooctane belongs to the class of flexible microemulsions, since the two hydrophobic chains are branched[1].



We experimentally determine the conductivity behavior along water dilution lines while keeping all parameters constants, varying only the proton to sodium ratio, i.e. the spontaneous curvature[2]. Confronting conductivity behavior observed along these different liens allows to identify and understand the condition of appearance of four completely different regimes of conductivity (I to IV) on the figure[3]. We will discuss and quantify the molar conductivity values in the four regimes.

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Multi-Component Self Assembled Molecular Electronic Thin Films – Towards New High Performance Thermoelectronics

Troy L. R. Bennett,[a] Xintai Wang,[b,c] Sophie Au-Yong,[b] Majed Alshammari,[b] Ahmad Almutlg,[b] Ali Ismael,[b,d] Luke Wilkinson,[e] Tim Albrecht,[f] Samuel P. Jarvis,[b] Lesley F. Cohen,[c] Colin J. Lambert,[b] Benjamin J. Robinson,[b] and Nicholas J. Long[a]

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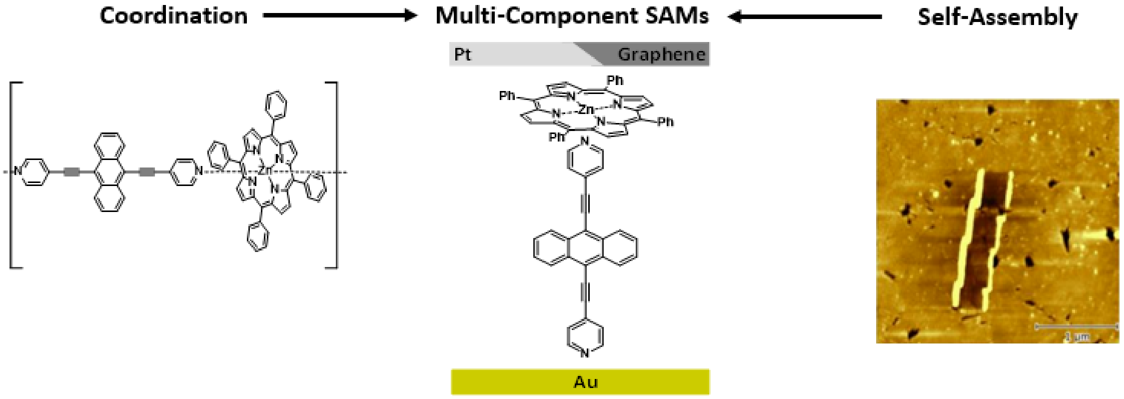
Abstract:

Waste heat is regarded as a low quality form of energy which is difficult to transform and utilise. The development of new techniques to recapture this energy are of high-importance, and organic materials have been widely studied for their thermoelectric properties i.e the conversion of heat into electricity via the Seebeck effect. In particular, self-assembled monolayers (SAMs) present an interesting opportunity within this context as these offer the potential for large-area, flexible, solution processable materials, that have well-defined structures and can take advantage of a number of molecule specific effects, such as tunability and quantum interference (QI).[1] Recently we have demonstrated that constructive QI can be scaled from single-molecules into SAMs, and can be effectively applied to boost both conductance and Seebeck coefficients. However these systems are still limited by their need for rigid-contacts between molecules and metallic-electrodes.[2]

Here we show that these design restrictions can be overcome by assembling multi-layered thin-film materials, by first forming a SAM and then taking advantage of its coordinative behaviour to deposit a second SAM on-top, boosting the Seebeck coefficients of our systems and promoting binding to graphene. These results were quantified through the use of AFM and XPS, and benchmarked against theoretical calculations. Our studies present an interesting avenue towards optimisation of the thermoelectric properties of SAMs via asymmetric interactions with terminal electrodes.[3]

References:



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(3) Manuscript in preparation.

Redox-controlled hybridization of electroactive foldamers

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Abstract:

Since 2000, foldamers have attracted the attention of chemists all over the world.[1] Mostly inspired by biomacromolecules, foldamers constitute a family of artificial oligomers that adopt well-defined conformations, which are stabilized by non-covalent interactions. These structures find numerous applications related to biology, molecular recognition,[2] catalysis,[3] or more recently, stimuli responsive materials.[4] Among the diversity of foldamer backbones few skeletons hybridize to form multiple helices.[5] The corresponding dynamics proved to be affected by parameters, such as temperature, concentration and solvent.[6] However, controlling this equilibrium in a reversible manner remained largely unexplored until recently. In this context, we currently explore the possibility to tune the hybridization abilities of foldamers through redox stimulations. This challenge was first tackled with tetrathiafulvalene-based foldamers endowed with five-pyridyl rings.[7] Now, our efforts are dedicated to the generalization of this strategy with longer oligomers and more importantly, on the extension of this concept to double helices made up of two complementary strands and called heteroduplexes.

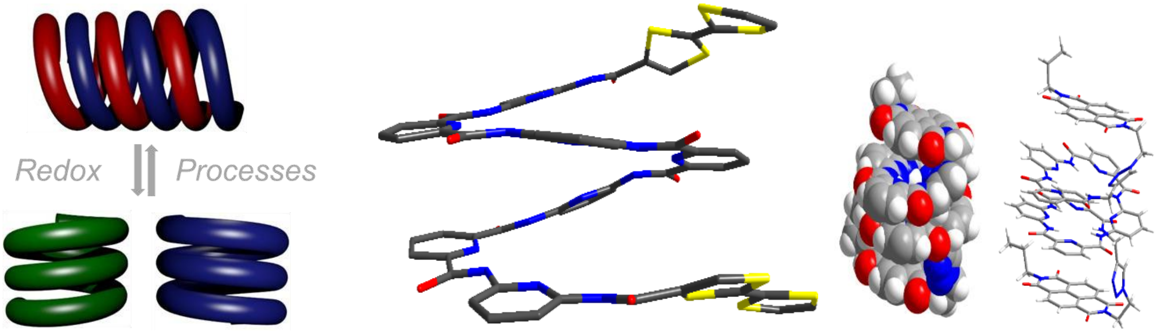

Figure 1. *left. Schematic representation of the redox-controlled hybridization of foldamers. Center. X-Ray crystal structure of a TTF-based oligopyridine dicarboxamide foldamer. Right. X-Ray crystal structure of a NDI-based oligopyridine dicarboxamide foldamer.*

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DNA Origami Self-Assembly For Lithography

Ludwig ROTSEN [a,b,*], Gaëtan BELLOT [b], Guido RADEMAKER [a], Raluca TIRON [a]

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Abstract:

Recent developments in DNA processing allow for the creation of unidimensional (1D), bidimensional (2D) or tridimensional (3D) nanostructures by means of DNA origami technology. These structures have nanometric precision and demonstrate high versatility, demonstrated by their use in fields as diverse as material science, nanomedicine and nanoelectronics. For nanoelectronics, research centered on the deposition and the immobilization of DNA origamis on mica or silica substrates. The DNA origami serves as an etch mask to transfer their motifs into silicon [1, 2]. Later, research extended to substrate-assisted self-assembly of DNA origamis on mica, to create highly ordered nanostructures [3]. The method is based on the exploitation of the interactions between the DNA origamis, the substrate and the divalent/monovalent cations.

The aim of this study is to create two square DNA origamis, which can self-assembled in 2D arrays by complementarity-shape directly on thermal SiO_2 substrates. The advantage of this method of self-assembly is that it exploits the low-energy π-π interactions present between square DNA origamis. Therefore, it is possible to create reversible hierarchical DNA nanostructures by increasing the Mg^{2+} concentration and controlling the temperature of the system [4]. Additionally, this reversibility offer the possibility to have potential spontaneous self-repairing properties in the 2D arrays as it has been demonstrated for the case of tubulin filaments [5]. I will present our latest results on the substrate-assisted self-assembly of these DNA origamis on thermal SiO_2 substrates. The 2D arrays created will be used as lithographic masks to make 2D silicon qubits arrays for quantum computing application.

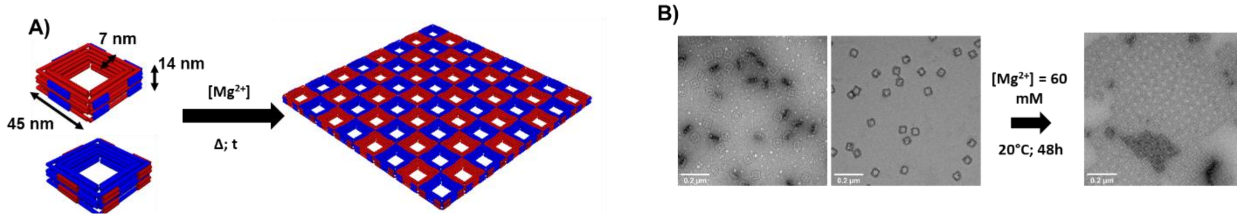

Figure 1 : A) 3D Modelization of the square monomers which can self-assembled by complementarity-shape in 2D arrays. B) TEM images of the complementary monomers and of a 2D array self-assembled with 60 mM of Mg^{2+} at 20°C during 48h.

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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"

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

Invited Speaker

Operation mechanism of Hyperfluorescence OLEDs

Chin-Yiu Chan, Yi-Ting Lee, Youichi Tsuchiya, Masaki Tanaka, Hajime Nakanotani, and

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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Hybrid Field Effect Transistor (HFET): A fully covalent transistor with a pi-conjugated organosilica

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Abstract: Here we demonstrate the use of novel organosilica materials embedding π-conjugated moieties as semiconductor into field effect transistors. The π-conjugated core chosen is [1]benzothieno[3,2-b] [1]benzothiophene (BTBT),[1] first functionalized with hydroxyl groups[2] and then modified with hydrolysable and cross-linkable triethoxysilyl moieties. After polycondensation, this compound forms a hybrid material composed of charge transport pathways as well as insulating layers (SiOx). However, overall, the material is found to be a semiconductor and can be incorporated into field effect transistors. Taking advantage of the solgel chemistry[3] involved here, we built Hybrid Field Effect Transistors that are fully cross-linked with covalent bonds.[4] Molecules are cross-linked to each other, covalently bonded to the silicon oxide dielectric and also covalently bonded to the gold electrode thanks to the use of an appropriate additional interfacial monolayer in between. This is the first report of fully covalent transistors. Those devices show impressive resilience against polar, aliphatic and aromatics solvents (even under sonication). This study opens the route towards a new class of hybrid materials to create highly robust electronic applications.

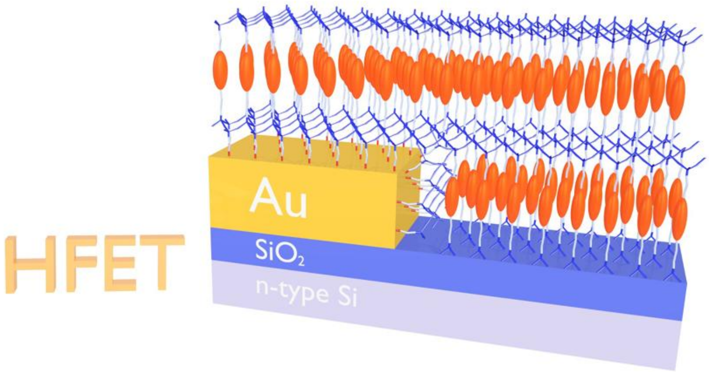

Figure 1: Hybrid Field Effect Transistors (HFET), First example of a field effect transistor based on an entirely reticulated organosilica active layer.

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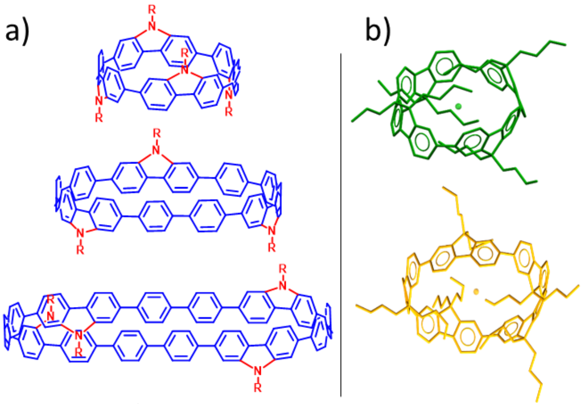
Nanohoop size influence in bridged cyclo-*para*-phenylenes

Cassandre Quinton,[a] Fabien Lucas,[a] Lambert Sicard,[a] Joëlle Rault-Berthelot,[a] Cyril Poriel[a]

[a]*Univ Rennes, CNRS, ISCR-UMR 6226, 35000 Rennes, France. Email: cassandre.quinton@univ-rennes1.fr*

Abstract:

Since 2008 and the synthesis of the first cyclo-*para*-phenylene (CPP),[1] which is the cyclic association of phenyl units *via* para linkages, hoop-shaped π-conjugated macrocycles possessing radially directed π-orbitals (so called "nanohoops") have been subject to intense research worldwide.[2-4] Compared to their linear counterparts, nanohoops possess unique electronic and structural characteristics.[5] In 2016, Nuckolls and co-workers have shown the several advantages of cyclic oligomers over corresponding linear counterparts in electronics devices.[6] In 2019, theoretical calculations have predicted the strong potential of CPPs as high mobility materials.[7] Since then, we showed that cyclo-2,7-carbazoles can be used as an active layer in an organic field-effect transistor (OFET) and provided a first benchmark in term of OFET characteristics for this type of cylindrical π-conjugated systems. We performed a detailed structure-properties-device performance relationship study of three cyclo-2,7-carbazoles bearing different alkyl chains on their nitrogen atoms, cyclo-2,7-fluorene and cyclo-para-phenylene in order to shed light on the impact of the bridge (presence, nature and substitution) in bridged cyclo-*para*-phenylenes.[8,9]



Structures of the studied nanohoops based on a) carbazole units, b) fluorene units

Considering the field of nanohoops, the influence of the hoop size on the electronic properties is probably the most fascinating feature.[2] However, if this has been deeply studied in the case of CPPs, it is far to be the case for the other nanohoop families. In the present work, we compare the structural, optical and electrochemical properties of several nanohoops displaying different sizes (3, 4 or 5 constituting units) within two families of bridged cyclo-*para*-phenylenes, the cyclo-2,7-carbazoles and the cyclo-2,7-fluorenes,[10] in order to shed light on the evolution of the properties upon size. The findings concerning the evolution of the frontier orbitals upon size could be used to design nanohoop-based semi-conductors with HOMO/LUMO levels fitting a desired application. Regarding the photophysics, the evolution of the absorption properties in solution upon size is specific to bridged cyclo-para-phenylenes whereas the evolution of the fluorescence properties follows the rules defined for CPPs. For all nanohoops, defining the evolution of their structural and electronic properties as a function of the hoop size is a crucial step in the understanding of these new generations of π- conjugated systems and their possible applications. This is the aim of this work.

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Determination of the Density-of-States in OLED Host Materials using Thermally Stimulated Luminescence

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Abstract:

Density-of-States (DOS) plays a central role in controlling the charge-carrier transport in amorphous organic semiconductors. The experimental determination of the DOS profile, however, is far from trivial. Several experimental techniques are used to probe the DOS of organic films, such as temperature-dependent space-charge-limited-current spectroscopy, UPS, inverse photoemission spectroscopy, Kelvin probe force microscopy, electrochemically gated transistor approach, as well as thermally stimulated luminescence (TSL). A clear advantage of TSL is that it is a purely optical and electrode-free technique. TSL originates from radiative recombination of charge carriers thermally released from the lower-energy part of the intrinsic DOS that causes charge trapping at very low temperatures.

In this work [1] we apply the low-temperature fractional TSL technique to determine the DOS of pristine amorphous films of organic light-emitting diode (OLED) host materials. The DOS width is determined for two series of hosts, namely, (i) carbazole-biphenyl derivatives: CBP, mCBP, and mCBP-CN, and (ii) carbazole-phenyl derivatives: mCP and mCP-CN. We find that the intrinsic DOS can be approximated by a Gaussian distribution, with a deep exponential tail accompanying this distribution in CBP and mCBP films. The DOS profile broadens with increasing molecular dipole moments, varying from 0 to 6 D, in a similar manner within each series, in line with the dipolar disorder model. This was confirmed by simulations that demonstrate a similar trend in the variation of DOS. The same molecular dipole moment, however, leads to a broader DOS of CP compared with CBP derivatives. Using QM/MM Molecular Dynamics simulations, it was attributed the difference between the series to a smaller polarizability of cations in CP derivatives, leading to weaker screening of the electrostatic disorder by induction. These results demonstrate that the low-temperature TSL technique can be used as an efficient experimental tool for probing the DOS in small-molecule OLED materials.

This work has received funding from EU Horizon 2020 Program through the Marie Skłodowska-Curie ITN 'TADF*life*' grant (GA no. 812872).

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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].

References:

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Quinonediimine ligands: from oligomeric coordination complexes in solution to molecular wires on surfaces

Simon Pascal,[a] Lucien Lavaud,[a] Hassib Audi,[a] Gabriel Canard,[a] Vijai M. Santhini,[b] Christian Wäckerlin,[b] Aleš Cahlík,[b] Jack Hellerstedt,[b] . Mendieta-Moreno,[b] Denis Jacquemin,[c] Pavel Jelínek,[b] Olivier Siri[a]

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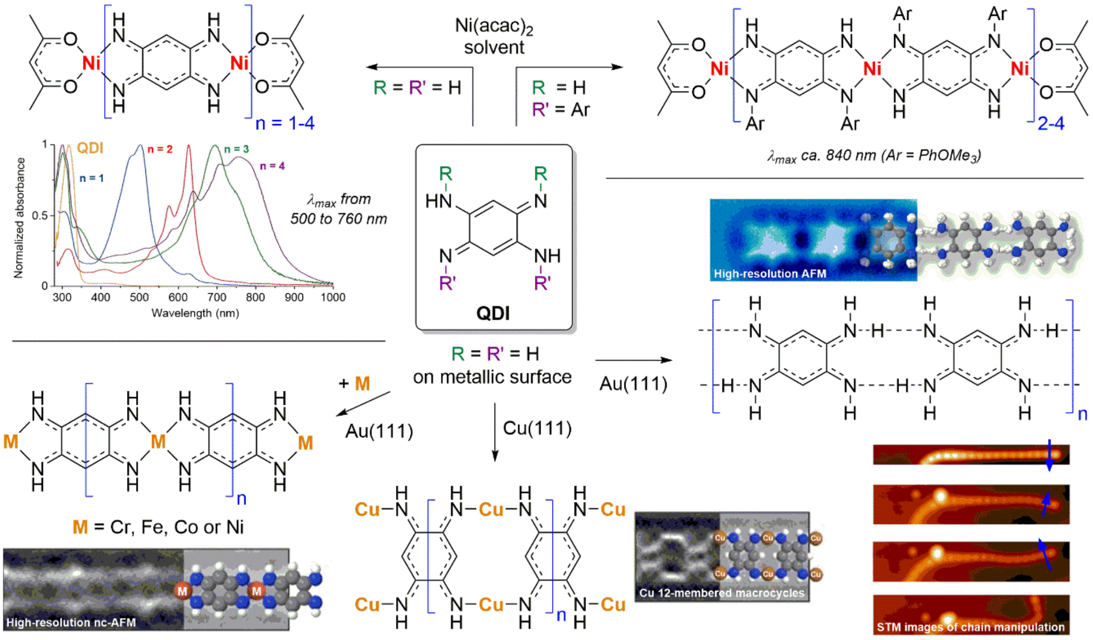
Abstract:

2,5-Diamino-1,4-benzoquinonediimine (QDI) stands as a versatile bis-bidentate and ditopic ligand for the preparation of coordination complexes featuring unusual optical or magnetic properties.[1] In solution, un/di-substituted QDIs allow to prepare extended and planar Ni(II) tapes whose absorption maxima directly depend on the length of the oligomers and can reach the near-infrared range.[2] Recently, on-surface synthesis of coordination polymers with QDIs under ultra-high vacuum conditions enabled the formation of flexible 1D π-d conjugated wires (M = Cr, Fe, Ni, Co, Cu) with lengths up to hundreds of nanometers.[3] This strategy also lead to unprecedented hydrogen-bonded assemblies of QDIs that exhibit π-conjugation along the chain due to concerted proton transfer and can be manipulated.[4]



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Graphene Meets Ionic Liquids: Fermi Level Engineering via Electrostatic Forces

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Abstract:

Graphene, a single layer of carbon atoms in a two-dimensional (2D) hexagonal lattice, showcases key properties suitable for electrode materials such as high specific surface area, good electrical and thermal conductivities.[1] Ionic liquids (ILs) are a class of molten salts that are entirely composed of ions. These liquids possess exceptional properties appropriate for electrolytes, such as high electrochemical window, electrochemical stabilities and extremely low vapor pressure. Graphene-based 2D materials are promising candidates for a number of different energy applications. A particularly interesting one is in next generation supercapacitors, where graphene is being explored as an electrode material in combination with ionic liquids as electrolytes. Because the amount of energy that can be stored in such supercapacitors critically depends on the electrode − electrolyte interface, there is considerable interest in understanding the structure and properties of the graphene/IL interface. Here, we present the changes in the properties of graphene upon adsorption of ILs and ILs – organic solvent mixtures using a combination of experimental and theoretical tools. For example, Raman spectroscopy reveals that imidazolium tetrafluoroborate ILs (CnMIM BF4) cause n-type doping of graphene, and the magnitude of doping increases with increasing cation chain length despite the expected decrease in the density of surface-adsorbed ions (Fig 1). Molecular modeling simulations show that doping originates from the changes in the electrostatic potential at the graphene/IL interface. The findings described here represent an important step in developing a comprehensive understanding of the graphene/IL interface.[2]

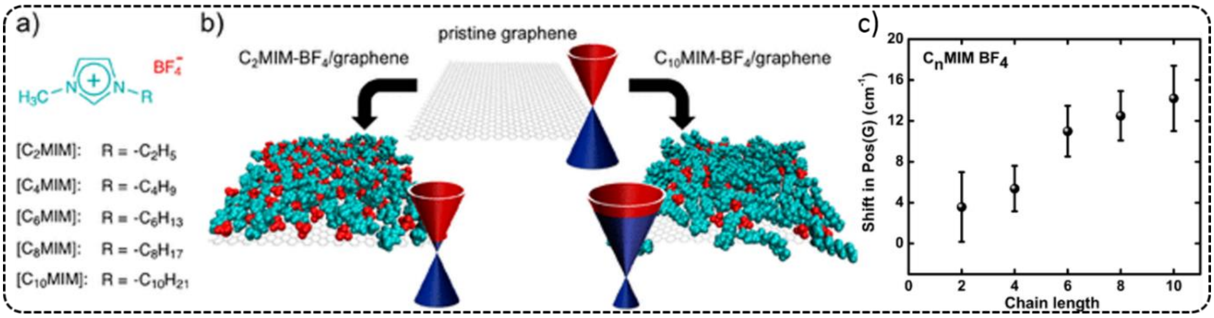

Figure 1: *(a) Molecular structures of the ILs employed in this study. (b) Scheme showing the influence of the adsorption of ILs with increasing chain length on the Fermi level of graphene. (c) Shift in Pos(G) versus the number of carbon atoms present in the alkyl chain on the imidazolium cation.*

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

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Abstract:

Perchlorotriphenyl methyl (PTM) radical is a stable persistent organic free radical with 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 alkyl, 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]. In order to expand its applications, we have modified single-walled carbon nanotubes (SWCNTs) via diazonium chemistry, being this, the first example of SWCNTs covalently modified with PTM radicals.[7]

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. [8] 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. [7]

Besides, other applications could be envisaged 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.

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Invited Speaker

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

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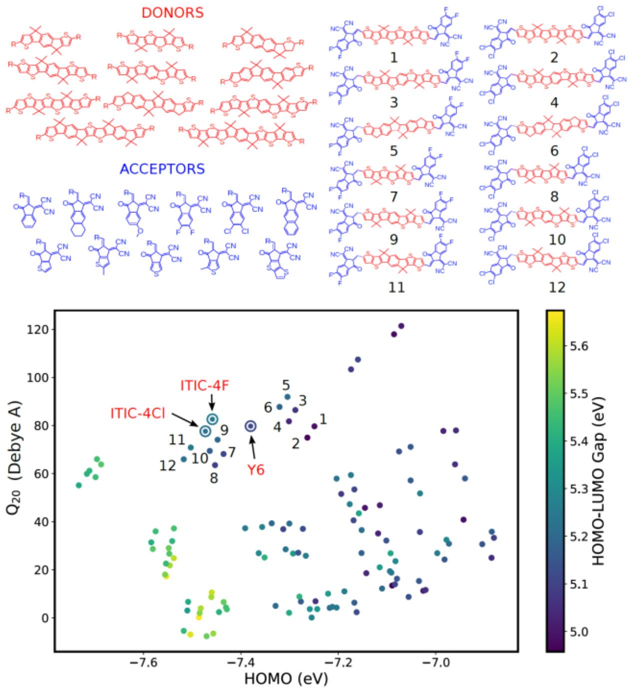
Abstract:

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

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From Memristor to Spinristor; Endohedral Metallofullerenes for Molecular Electronics

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Abstract:

Employing multi-scale *in silico* modeling we propose molecular memristors on the basis of endohedral fullerenes, encapsulated with polar molecules of general type MX (M: metal, X: non-metal) to be used for data storage and processing.[1] We demonstrate for MX@C_{70} systems that the relative orientation of enclosed MX with respect to a set of electrodes connected to the system can be controlled by application of oriented external electric field(s). We suggest systems with two- and four-terminal electrodes, in which the source and drain electrodes help the current to pass through the device and help the switching between the conductive states of the memristor via an applied voltage. The gate electrodes then assist the switching by effectively lowering the energy barrier between local minima via stabilizing the transition state of switching process if the applied voltage between the source and drain is insufficient to switch the MX inside the fullerene. Using non-equilibrium Green's function combined with density functional theory (DFT-NEGF) computations, we further show that conductivity of the studied MX@C_{70} systems depends on the relative orientation of MX inside the cage with respect to the electrodes. Therefore, the orientation of the MX inside C_{70} can be both enforced ("written") and retrieved ("read") by applied voltage. The studied systems thus behave like voltage-sensitive switching molecular diodes, that is a reminiscent of a molecular memristor. Further, we discuss possibility of making a spin-filtering memristor, spinristor, using the similar systems.[2]

Acknowledgements

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Theoretical Design of Multi-State Multi-Addressable Multi-Functional Molecular Switches

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Abstract:

This paper illustrates how theoretical chemistry methods are developed and enacted to help designing multi-state (more than 2), multi-addressable (more than one stimuli; *e.g.* light irradiation, pH/redox potential changes), multi-functional (linear and nonlinear optical properties) molecular switches. The targeted molecules are built from benzazolooxazolidine (BOX) units, which are combined with 1°) different kinds of organic/organometallic donor units, with 2°) other switchable units like diarylethene, or simply 3°) linked together to create diBOX or triBOX derivatives. To study these switches in solution as well as in the form of self-assembled monolayers, the theoretical chemistry methods encompass 1°) quantum chemistry approaches, mostly density functional theory (DFT) and time-dependent DFT, of which the reliability has been substantiated by comparison with high-level wavefunction methods and 2°) molecular dynamics simulations using re-parameterized force fields to describe the π-conjugated frameworks because the optical properties are much sensitive to the molecular geometry. Our work focuses on those molecular switches presenting contrasts of second harmonic generation (SHG), a second-order nonlinear optical (NLO) phenomenon that is probed in solution by using the hyper-Rayleigh scattering technique. From an application perspective, NLO molecular switches present the "read without erase" advantage while the SHG response is much sensitive than the linear ones.

This paper shows how large SHG contrasts can be achieved and how they are related to structural changes as well as to the corresponding linear optical responses (usually analyzed by UV/vis absorption spectroscopy so that the SHG response is analyzed within few-state models). Besides the molecular properties (including also the change of free enthalpy upon (de)protonation/redox reactions), the presentation discusses the role of the surrounding (solvent, monolayer) and how it can be modelled (polarizable continuum model *versus* explicit solvation; polarization and local field effects).

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Multi-Step Fisher-Lee: A new tool to predict transport mechanism transition in molecular junctions.

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Abstract:

In the past decade, research groups took advantage of the progress on the growth of molecular junction to explore the electronic transport properties in different regimes (non- resonant tunneling, hopping, resonant-tunneling, etc...) by measuring their electric properties while varying the molecular length[1]. While the existing theories correctly describe the transport in the non-resonant tunneling regime (*i.e.* for short molecules), there is no reliable model to connect the regimes to each other[2]. Here, we present a new methodology based on the Non-Equilibrium Green Function (NEGF) combined to the Fisher-Lee formalism[3] within a semi-classical approach, to predict the transport mechanism transition between the non-resonant tunneling and the following regimes. This new approach labeled Multi-Step Fisher-Lee (MSFL)[4] consists in comparing a direct tunneling mechanism to a multistep tunneling in the Fisher Lee formalism. We have applied it to a wide range of molecular junctions and the obtained results are in a good agreement with experimental measurements. This work opens perspectives for a better understanding of the transport mechanism in molecular junctions.

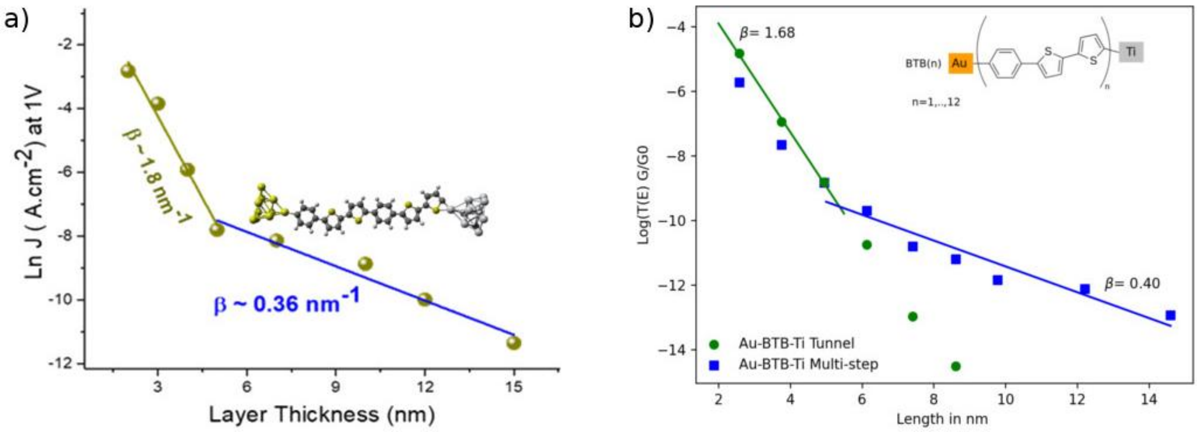

Figure: Comparison of a) experimental[5] results and b) our results using the MSFL method for the molecular junction Au-BTB-Ti.

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Invited Speaker

Can Protein Electronic Conduction be a Quantum effect?

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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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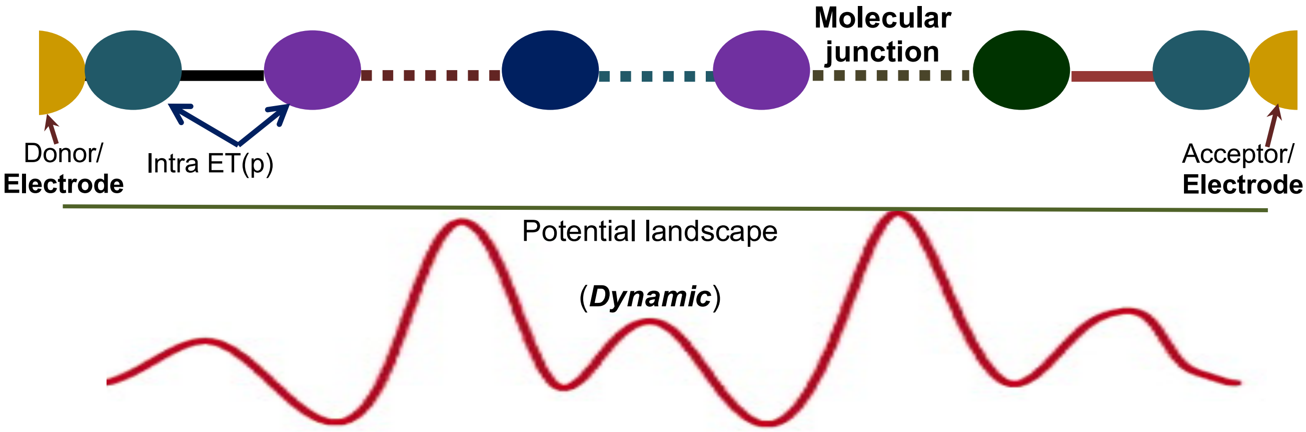

Figure: Schematic of protein junction, depicted as arrangement of amino-acids and cofactors, (TOP) and a snap-shot (< psec) of the electrostatic potential (BOTTOM); from ref. 1, to be referred to as the source.

Nanostructured Carbon Materials for Bioelectrochemical Applications

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Abstract:

The outstanding properties of nanostructured carbon such as carbon nanotubes or graphene made them a widely used material as electronic or electrochemical transducer in biosensor devices. Carbon nanotubes (CNTs) possess the outstanding combination of nanowire morphology, biocompatibility and electronic properties. Furthermore, their ease and well-documented organic functionalization brings new properties to nanostructured electrodes such as specific docking sites for biomolecules. Moreover, CNT films exhibit a high electroactive surface area due to the natural formation of highly porous three-dimensional networks, suitable for the anchoring of a high amount of bioreceptor units, leading consequently to improved sensitivities. Furthermore, the controlled formation of porous structures with reproducible identic morphology led to reliable high performing label free impedimetric immunosensors [1]

Since several years, monolayer graphene and related 2D carbon materials are shown as promising alternative to CNTs. However, graphene should be seen as complementary material to CNTs like the plasmonic coupling with gold surfaces in SPR biosensors [2].

Nanostructured carbon also became essential electrode materials for energy storage or harvesting. In particular, enzymatic glucose biofuel cells have gained wide attention due to the possibility to harvest energy from complex media like body fluids. Further advantages are that the biological energy production can take place at neutral pH and at room temperature by converting a wide range of sustainable (bio)-fuels. However, the main drawback for enzymatic biofuel cells are their limited power output and operational life time. One of our proposed design of bioelectrodes for enzymatic biofuel cells is based on free standing carbon nanotube pellets that allows high enzyme loading in a protective environment with satisfying stabilities [3]. Other carbon nanotube shapes like buckypapers were functionalized and tested for the energy conversion of glucose [4]. Some alternative approaches to optimize the electron transfer [5] is presented .

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Exploring Memristive Squaraine Nanowire Networks: Programmable Multi-Level Memory Behaviour for Neuromorphic Applications

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Abstract:

Typically, the demand for faster, cheaper, more efficient computing has been answered by device miniaturisation. However, device down-scaling (particularly that of transistors) is fast approaching the atomic scale, resulting in a gulf between the computational efficiency required by data scientists and hardware capacity available from conventional computing based on the von Neumann architecture and binary operations.[1] Artificial electronic synapse (e-synapse) devices are necessary in order for the effective implementation of artificial neural networks (ANNs) in hardware / machine learning operations to occur.[2] Organic memristors can provide the functionality required to meet these computational demands by providing multi-level memory coupled with high-density integration, as well as possessing all of the advantages inherent to organic materials such as flexibility and biocompatibility.[3] Memristors are two-terminal resistive switches which can encode information in the form of programmable internal resistance, the evolution of which can be modulated by the history of its external stimuli.[4] Memristors offers much greater memory density than typical devices by enabling 'multi-bit' memory, as well as facilitating the co-location of memory and logic operations, overcoming the energy- and time-expensive separation between memory and computation execution.[5]

Herein we demonstrate a self-assembled analog resistive switching nanowire network with programmable multi-level memory based on 2,4-bis[4-(N,N-diisobutylamino)-2-6-dihydroxyphenyl]squaraine (SQ), a small-molecule organic semiconductor. The device shows the typical pinched hysteretic *I-V* loop of a memristor with gradual changes in conductance upon successive sweeps, akin to the synaptic weight update processes in the human brain. The memory retention is shown to decay to its original state within a relatively short time in the absence of external voltage application, which is satisfactory for neuromorphic computing applications such as online learning where the synaptic weight values can be stored elsewhere following the training process.[2] This time-dependence enables short-term plasticity functionality to be demonstrated (paired-pulse facilitation and post-tetanic potentiation). Potentiation and depression cycles are shown to exhibit linear and symmetric conductance tuning, a key requirement for implementation of neuromorphic computing. Furthermore, short-term memory to long-term memory conversion is demonstrated through repeated sequences of voltage pulses. Overall, SQ nanowire networks appear to present attractive properties that could enable the successful embedding of organic nanowire-based ANNs directly in hardware circuits.

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Amyloid fibers for bioelectronics: HET-s(218-289) used for brain-machine interfaces

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Abstract:

Amyloid fibers were first known for their involvement in neurodegerative diseases (Ross and Poirier 2004). But overall, we learned, in the last decade, that they support predominantly functional mechanisms in a wide range of organisms (Levkovich, Gazit, and Laor Bar-Yosef 2020). Indeed, their properties make them a promising challenger to form a whole new kind of biomaterials. Easily synthetized and tunable, with high stability and mechanic resistance, amyloid fibers exhibit characteristics never gathered in one component.

Our study focused on HET-s prion domain (218-289), which is a fungus (*podospora anserina*) protein forming high aspect ratio (>2000) amyloid fibers (Doussineau et al. 2016). As a recombinant protein, we produced and purified it using biochemistry techniques and then studied its electrical properties. Only by its protonic conduction, relying on Grothuss mechanisms, we showed that it was able to transmit artificial pulses as short as 500ns with an amplitude of only 100mV with high reliability.

To go further, we performed *in vitro* neuronal activity recordings, using multielectrode array (MEA), on hippocampal primary neurons, grown on HET-s(218-289) hydrogel substrate. After 30 days, neurons have developed normally, showing every sign of good health, notably action potentials train spikes reaching few dozen microvolts. We also realized *in vivo* biocompatibility experiment in rats; no cytotoxicity appeared even after several months. Such results pave the way for new electrodes and/or new-generation electrode coating relying on materials from the same origin that the recorded objects. Added with the possibilities of functionalization (Altamura et al. 2017), one can imagine even more complex recording coatings for innovative brain-machine interfaces

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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

Invited Speaker

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

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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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Support from Institute for Basic Science (IBS-R027-D1) is gratefully acknowledged.

Probing local switching currents induced by polarization reversal in an organic ferroelectric thin film

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Victor Da Costa

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Abstract:

Ferroelectric devices offer multiple advantages over other materials devices implementations, from low-energy information encoding to neuromorphic computing architectures [1, 2, 3, 4]. However, a precise understanding of how the polarization reversal occurs remains lacking. As electronic devices are shrunk to the nanoscale, their properties become more and more sensitive to defects, and to the physical properties that emerge at the interface, where different materials interact.

We demonstrate the successful detection of tiny ferroelectric switching currents of a few pico-amperes of magnitude originating from a nanoscopic region consisting of only a few grains in an organic ferroelectric thin film without any top electrode. By detecting the strain response of the region when submitted to the applied bias, we prove that the detected currents are indeed due to the polarization reversal occurring in the grains. The measurement of switching currents allows us to estimate the polarization charge density in a nanoscopic region (~300x300 nm2). As the ferroelectric system, we chose polycrystalline films of Croconic Acid (CA) [5, 6, 7] grown on Cobalt substrate in ultra-high vacuum environment, and performed in-situ spectroscopic measurements with a metallic tip in contact with the top surface. From these experiments, we report a nanoscopic polarization charge density of ~10 µC/cm2 which is of the order of the reported values of CA crystals [8]. For the sake of generality, we also extended the approach to a commonly studied inorganic ferroelectric material, $BiFeO_3$.

We are working towards switching current detection from even smaller areas; from a single grain or part of a grain in a polycrystalline film. The possibility to measure switching currents originating from the polarization reversal of single ferroelectric grains will pave the way towards understanding the fundamental ferroelectric properties at the granular level in continuous thin films. An understanding of the associated dynamics and of the kinetics of polarization reversal processes at granular level will lead to a better control over the switching processes in ferroelectric-based nanoelectronic devices.

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Light-matter interaction at the single-molecule level probed with STM

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Abstract:

Light-matter interaction plays a crucial role in the quantum properties of light emission from single molecules. They are usually probed using optical methods, which are, however, spatially limited by diffraction to a few hundred nanometers. On the other hand, scanning tunneling microscopy (STM) routinely reaches picometre spatial scale. Recent works have shown that the tunneling current of an STM can be used to excite the intrinsic luminescence of individual molecules enabling light-matter interaction investigations with unprecedented resolution. Processes that can be addressed involve charging, dipole-dipole interactions or energy transfer between individual chromophores.

Here, we study STM-induced luminescence from phthalocyanine molecules adsorbed on a few-monolayer NaCl film epitaxially grown on Ag(111) substrate. We show how the atomically-confined electromagnetic field at the STM tip apex acts as a "picocavity" for localized plasmons and both enables optical studies with atomic-scale precision and interacts with the emitter [1]. Profiting from that resolution, we investigate a critical mechanism in the photosynthesis process – resonant energy transfer in multichromophoric architectures. We use individual phthalocyanines as ancillary, passive or blocking elements to promote and direct resonant energy transfer between distant donor and acceptor units. Such an approach constitutes a powerful model to study the role of the relative dipole orientation, distance and chemical nature of the chromophores on the efficiency of the energy transfer [2].

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

Affinity driven ion exchange EG-OFET sensor for high selectivity and low limit of detection of Cesium in seawater

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Abstract:

The detection and quantification of Cs^+ in aquatic media are an environmental safety and public health matter, so far limited by the lack of rapid, low cost, low limit of detection and selective analytical tools. Herein we demonstrate the efficient fabrication of a novel electrolyte-gated organic field-effect transistor sensor for the Cs^+ detection in seawater based on the combination of two ultra-thin layers namely poly(3-hexylthiophene) as semiconductor and a single lipids monolayer as dielectric [2,3]. The latter is end-capped with a specific Cs^+ probe based on a calix[4]arene benzocrown ether to ensure the selectivity.

Cs^+ sensing experiments were performed in various conditions, including the presence of competitive ions and/or solutions with very high ionic strength. Interestingly, we clearly evidence that by controlling affinity driven guest/host ion exchange, one can lift the general problem of selectivity encountered in all FET-based ion sensors, reaching selectivity even in highly complex analytes, such as phosphate buffered saline solution or seawater.

Also our ultra-thin transistor structure exhibits, a limit of detection at the attomolar level which corresponds to a 5 folds' magnitude lower than Inductively Coupled Plasma Mass Spectroscopy, the most commonly used technic today (Fig. 2). Such low limit of detection cannot be explained solely by the change in surface potential induced by the capture of ions by the probe; instead we suggest a reorientation of the dipoles moments at the probe level that may propagate on a large distance leading to an enhancement of the surface potential change induced by an initial ion/probe complexation event.

These results pave the way to a generalized monitoring of ions in complexed analytes.

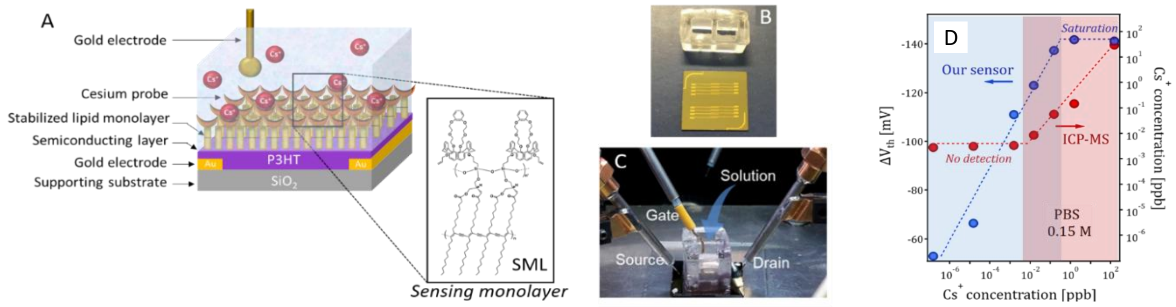

Figure 2 : A) EG-OFET sensor design based on ultra-thin layers of P3HT and engineered lipid monolayer as semiconducting and dielectric materials respectively. The Cesium probe is a calix[4]arene benzocrown ether grafted to the lipid monolayer through a triethoxysilane groups. B) Picture of a chip containing 8 transistors mounted in parallel. C) Picture of the set-up for electrical measurements. D) Comparison of the performances of EG-OFET sensor (in blue) with ICP-MS based detection (red).

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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Building UniMolecular Scaffolding for Electronic Devices

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Paul J. Low,[5] Pilar Cea,[1,2,6] José Luis Serrano,[1,4] Santiago Martín[1,2,6]

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Abstract:

It is well known that many properties of advanced materials are related with a well-organized internal structure.[1-2] In this context, the construction of the next generation of electronic and optical devices will require a spatial orientation and control of the molecular arrangement of the functional molecules.[3] Although unimolecular electronics are already a reality, these are not consistent between themselves and to control the precise geometry at the molecule–metal contacts is one of the long-standing challenges in single-molecule electronics.[4] Therefore, to fabricate multiple unimolecular devices in a parallel way is still a remaining challenge.[5] Here, a controllable, tuneable, versatile and integral layer-by-layer (LbL) strategy to build a large-scale unimolecular scaffolding in a parallel way has been developed. This strategy consists in combining successive self-assembly layers of a substituted metallic porphyrin and a functional molecule, which is located in a defined position strictly normal to the substrate, spaced out from each other and keeping a 1:1 stoichiometric ratio through an 'electrical' contact (Figure 1). This strategy allows to modulate the structure of the final scaffolding by varying the functional molecule depending on the searched application; that is, extending this strategy to the preparation of more complex large-scale unimolecular devices. Thus, we hope this innovative layer by layer strategy offers new nanotechnological applications, since offer several exciting potential advantages, including suppression of in-plane transport, access for a wide range of functional wires, or free volume for electromechanically operated switches.

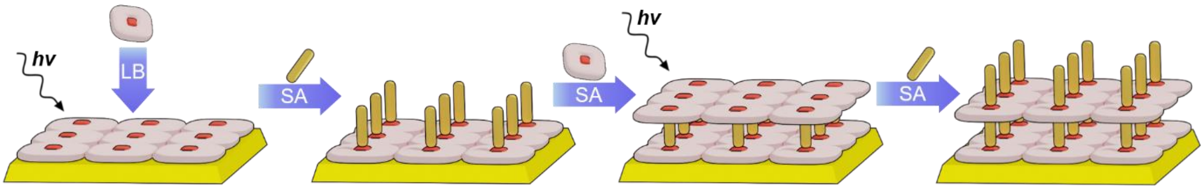

Figure 1. Scheme of the strategy followed to build layer by layer a large-area unimolecular scaffolding device.

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Bis-Acridinium Tweezers and Cyclophanes: Supramolecular Self-Assemblies, Self-Sorting and Multi-Switching Properties

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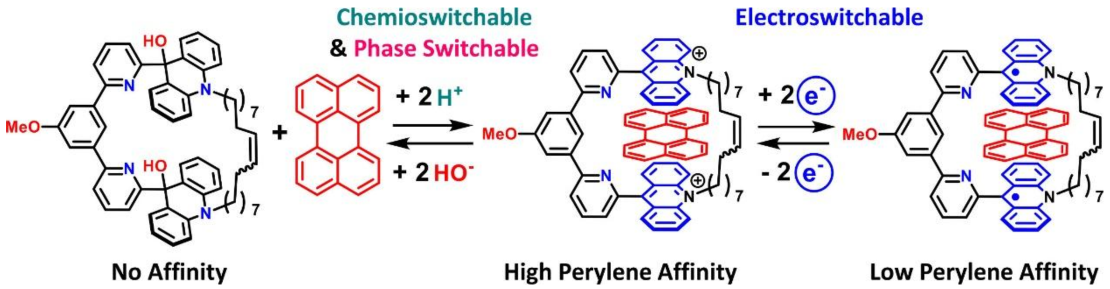
Abstract:

In Nature, the high degree of organization allows the formation of sophisticated assemblies (double helical structure of DNA, G-quadruplex secondary structures, etc.) able to perform advanced functions (modulation of reactivity, movement, etc.). In such complex mixtures, the organization is governed by selective molecular recognition and self-assembly processes[1] relying on weak interactions (hydrophobic, hydrogen-bonding, van der Waals, and π-π stacking interactions). Consequently, a growing interest in elaborating self-assembling systems has emerged in order to prepare functional synthetic systems in a simple and reliable manner.

We recently reported bis-acridinium receptors able to bind guest molecules.[2] Based on molecular tweezers and their cyclophane analogues, two acridinium recognition units linked by a semi-rigid spacer are pre-organized to bind a variety of aromatic guests. The acridinium recognition units are unique multi-responsive building blocks (electrochemically and chemically switchable) able to interact with electron rich guests.[3] Surprisingly, this class of bis-acridinium receptors exhibit i) self-complementary behaviors leading to the formation of entwined dimers,[2a] ii) narcissistic self-sorting as well[2b] as iii) π-donor/π-acceptor host-guest behaviors.[4] In addition, the multi-switching properties of these bis-acridinium receptors were investigated to alter the recognition events and were also studied as a selective phase transfer agent of perylene in perfluorocarbons.



Self-Assembly processes and Switching Properties of a Molecular Cyclophane bearing two Acridiniums.

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3 H.-P. Jacquot de Rouville, J. Hu, V. Heitz, *ChemPlusChem*, **2021**, *86*, 110–129.

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Fabrication and Characterization of 2D Metal-Organic Network on Weakly Interacting 2D Materials

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Abstract:

The fabrication of atomically precise structures with designer electronic properties is currently being vigorously pursued within condensed-matter physics and materials chemistry research communities [1]. Over the past two decades, low-dimensional metal-organic networks (MONs) with various atomically precise lattice structures have been fabricated on coinage metal surfaces [2]. Recently, our group has synthesized and characterized several two-dimensional (2D) MONs on the weakly interacting substrates under ultra-high vacuum (UHV) conditions using low-temperature scanning tunnelling microscopy (STM) and spectroscopy (STS) [3-5]. We demonstrate a successful synthesis of a large-scale monolayer Cu-dicyanoanthracene (DCA) network that can grow across the terrace of an epitaxial graphene surface [4]. The ordered DCA_3Cu_2 network shows a structure combining a honeycomb lattice of Cu atoms with a kagome lattice of DCA molecules. Combing the STM/STS data with density-functional theory (DFT) results, we confirm that a kagome band structure is formed in the 2D MON near the Fermi level. We demonstrate access to multiple molecular charge states in the 2D MON using tip-induced local electric fields, which highlights the role of electron-electron interactions that are likely to give rise to exotic electronic properties. Furthermore, to realize the exciting prospect of truly designer materials, it is important to demonstrate MOF synthesis on other 2D substrates. Here, I will also discuss our recent efforts of synthesizing metal-organic network on $NbSe_2$, which extends the synthesis and electronic tuneability of 2D MOFs beyond the electronically less relevant metal and semiconducting surfaces to superconducting substrate [5]. We expect that a similar strategy can be applied to the development of emerging quantum materials.

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2D host–guest supramolecular chemistry for an on-monolayer graphene emitting platform

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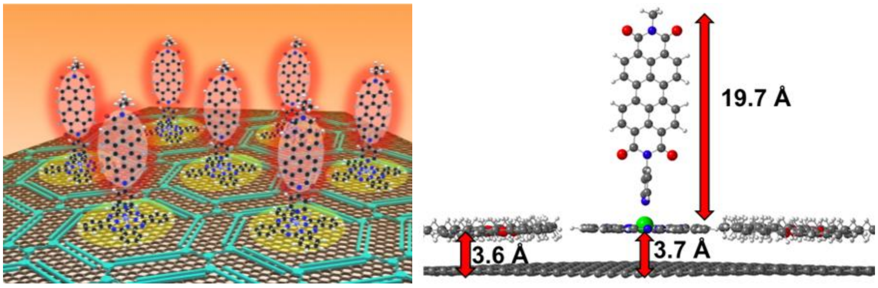
Abstract:

Electronic decoupling of molecular chromophores from graphene to preserve their optical properties with the objective to elaborate light-responsive hybrid system for new electronic and optoelectronic nanodevices remains largely unexplored.[1]

Here, we demonstrate for the first time an easy-to-implement strategy that successfully tackles the electronic decoupling issue.[2] Graphene-confined supramolecular host-guest recognition is used to elaborate an emitting hybrid platform. This noncovalent functionalization approach, based on two-dimensional (2D) host-guest supramolecular chemistry, enables immobilization of emitting 3D guest molecules into a 2D self-assembled porous template. It is shown that the cavities of an on-monolayer graphene nanoporous self-assembled network are able to trap zinc phthalocyanine (ZnPc) molecules coordinated to an appropriately designed emitting axial ligand (pyridine-functionalyzed perylene tetracarboxydiimide (Py-PTCDI)). As a result, the well-controlled graphene-chromophore and inter-chromophore distances combined with the mastered chromophore orientation perpendicular to the substrate, allow the elaboration of an emitting graphene-based hybrid system with the same features as the single molecular emitter, demonstrating the preservation of its intrinsic electronic properties. Furthermore, an in-depth modelling study confirms the weak interaction between the out of plane emitting moieties and the monolayer graphene.

Therefore, contrary to current photo-active graphene systems that take advantage of the direct electronic interaction (quenching) between the photo-responsive moieties and the graphene, our decoupling strategy that retains the molecular electronic properties is promising to create on demand innovative light-responsive graphene-based devices in nanophotonics and optoelectronics.



Sketched and side view of the modelled system made of a graphene layer, covered with ZnPc:Py-PTCDI emitting guest molecules trapped in the supramolecular self-assembled nanoporous host network.

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Redox state-modulated electron transport properties of polyoxometalates at the nanoscale

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and Dominique Vuillaume.[a]

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Polyoxometalates (POMs) are nanometric molecular oxides with remarkable redox properties that can be explored in the context of advanced components [1-3]. We propose to develop scalable functionalities in 2D nanomaterials based on POMs (2D-PN, 2D POM Network) "programmable/switchable" on demand thanks to the multifunctional properties of these molecules (e.g. multiredox states). The first objective is to prepare compact and dense monolayer of POMs on a metal substrate to assess their electron transport (ET) properties. Here, we report the ET properties of those POMs (here $[PMo_{12}O_{40}]^{3-}$ and $[NaP_5W_{30}O_{110}]^{14-}$) in their different redox states using self-assembled monolayers (SAM) and conductive-AFM (Figure 1). For both molecules, we clearly observed an increase of the conductance for the reduced states which is related to a decrease of the energy of the molecular orbital involved in the transport though the metal/POM/metal junction : from ≈0.65 eV to ≈0.43 eV for PMo_{12} and from ≈0.44 eV to ≈0.31 eV for P_5W_{30}. We tentatively ascribe this feature to a change from a LUMO mediated ET to a HOMO mediated ET after reduction (ab-initio calculations in progress). Then, we successfully fabricated multi-connected (6 electrodes) hybrid 2D-PN with $[PMo_{12}O_{40}]^{3-}$ and Au nanoparticles (Figure 2) and we measured their ET revealing large variability in the 2D-PN. Preliminary low-frequency noise and high-harmonic generation measurements will be used to discuss the possible use of these 2D-PN within the global framework of the physical implementation of a neuromorphic reservoir computing system with nano-objects (CNT, nanoparticles, molecules, atomic switches).[4-7]

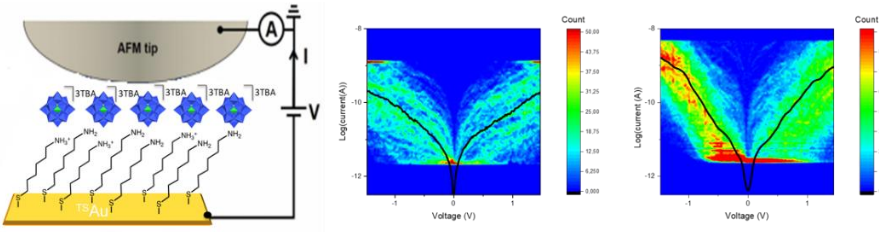

Figure 1 : General scheme of the electronic transport characterization by C-AFM of the $[PMo_{12}O_{40}]^{3-}$ electrostatically deposited onto alkylamine SAM functionalized gold surface and histogram of the current-voltage curves (I-V) in oxidized state (left) and after one electron reduction (right).

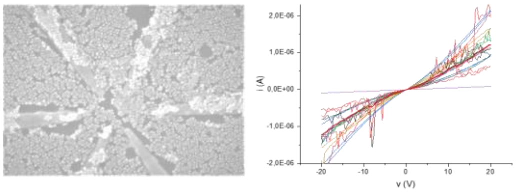

Figure 2 : SEM images (left) and current-voltage curves (I-V) (right) of fabricated multi-connected hybrid 2D-PN with $PMo_{12}O_{40}$ and Au nanoparticles

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Invited Speaker

Redox molecular junctions and thermal effects

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[b] *School of Chemistry, Tel Aviv University, Israel.*
Email: anitzan@sas.upenn.edu

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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Memory Nanodevice Based on Zn-MOF-74:
A Molecular Dynamics Study

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Abstract:

A two-level system based on C_{60}^{-}@Zn-MOF-74 is investigated by molecular dynamics simulation to explore an application as memory nanodevice. An external electric field triggers the displacement of C_{60}^{-} and defines the status of the system: bit 1 or 0.

The crystal structure of Zn-MOF-74 allows to achieve the high memory elements density and high switching speed. Zn-MOF-74 has one dimensional well-defined pores, which size is big enough to contain the C_{60} ion. There are two groups of electrodes, presented by (6,6) nanotubes. The structure of the system is shown in Figure 1.

The nanodevice has outstanding data **throughput rate about 27 Gbyte/s** and **high memory elements density - 106 Tb/inch^2** [1].

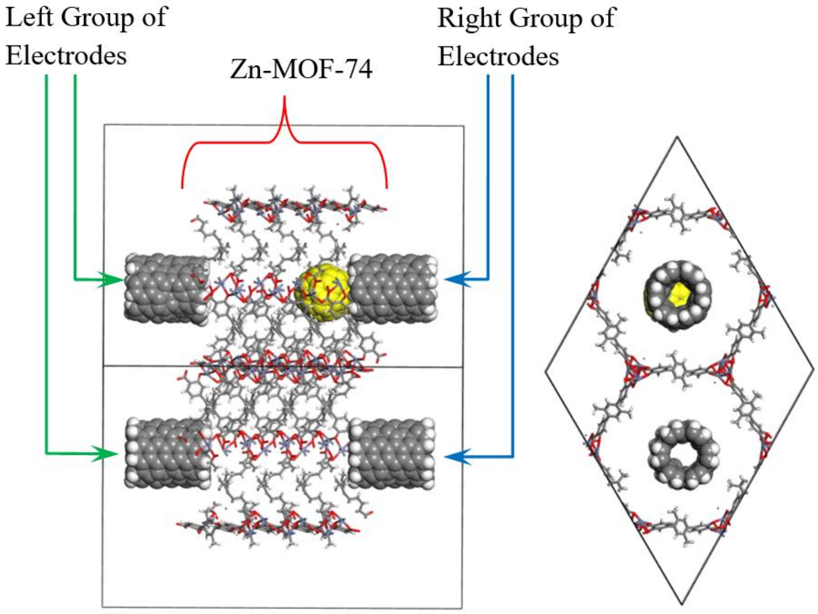

Figure. 1. Element of memory nanodevice, which consists of C_{60} ion (highlighted by yellow), which is enclosed in channel of Zn-MOF-74 with left and right groups of electrodes - carbon nanotubes (6,6).

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Looking for structure/property relations in OPV systems: a multi-level computational approach

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Abstract:

Organic electronics is set to become a major focus of academic and industrial research as it touches a diverse array of important technological fields spanning energy production and storage, computing and consumer electronics. The promise held by organic materials can be delivered if protocols able to speed up materials search are developed. The role of computational material modelling is therefore fundamental. The goal is to predict the relevant properties of a material at the molecular level with the appropriate inclusion of the environment, which may severely affect the performance by suppressing certain mechanisms or by promoting some others not displayed in isolated systems. Only an approach able to include an adequate description of the molecular surroundings allows, in principle, a reliable prediction of most macroscopic properties relevant to the envisioned application. The case of organic photovoltaics (OPV) is emblematic, since it requires an accurate molecular modelling of the electronic structure of the materials (donor and acceptor) at both ground and excited electronic states, as well as the modelling of the effects of short- and long-range interactions on this structure modulated by the morphology of the system.

In this context, we have developed throughout the years, a multi-level computational protocol which allows the prediction and rationalization of a number of key parameters (such as absorption spectra, structural features, hole/e^- transport efficiencies) for photoactive molecules used in OPV set in a variety of environments (solution, donor-acceptor interfaces, thin-films, crystals). The efficacy of the protocol will be illustrated by presenting its applications to a wide range of materials and conditions found in OPV devices, including photoactive polymers [1], small-molecule donors [2,3], molecular dyads for single-material solar cells [4] and non-fullerene acceptor/donor interfaces [65.

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Molecular design of semi-conducting metal-organic framework films

Mariana Kozlowska,[a] Mersad Mostaghimi,[a] Lars Heinke,[b] Ritesh Haldar,[b] Christof Wöll,[b] Wolfgang Wenzel[a]

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[b]Karlsruhe Institute of Technology (KIT), Institute of Functional Interfaces (IFG), Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany

Abstract:

Electronic properties of organic semiconductors (OSC) highly depend on the structural assembly of molecules and their vibrational flexibility in a material. These determine the microscopic intercommunication between the electronically active sites, resulting in a materials conduction. In most cases, aggregation of OSC is hard to control and a multitude of assembly possibilities occurs. Here, we have employed a metal-organic framework (MOF) type of crystalline assembly strategy to engineer the arrangement of the spiropyran photoswitches and functionalized pentacene-based semiconductors incorporated at controlled positions with defined intermolecular distances in MOFs, and demonstrated the change of the electronic and spectroscopic properties of molecules and films towards assembly in the spatially ordered MOF structure.

Based on our previous proof-of-principle study on spiropyran embedded in MOFs [1], showing for the first time the remote switching of the electric conduction of a MOF material, we used the combination of quantum mechanics and molecular mechanics approaches to design new MOF candidates with conductance properties that can be reversibly changed by light. With the implemented temperature-dependent dynamics of the molecules in a material, the charge carrier mobilities, considering both band-like transport and the Marcus charge hopping were obtained. A thorough quantum mechanical investigation allows identifying localized frustrated rotations of the pentacene cores as the reason for the breakdown of band transport [2]. It gives perspectives for realization of the highly anisotropic conduction with oriented photosensitive conduction highways.

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This research was funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) under the Coordination Networks: Building Blocks for Functional Systems DFG Priority Program 1928 and the Germany Excellence Strategy via the Excellence Cluster 3D Matter Made to Order (grant no. EXC-2082/1-390761711). We acknowledge the support by the Virtual Materials Design initiative (Virtmat) funded by KIT. M.K. acknowledges funding by the Ministry of Science, Research and Art of Baden-Württemberg (Germany) under the Brigitte-Schlieben-Lange-Programm.

Invited Speaker

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

Dominique Vuillaume

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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].

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[11] *Exploring thermoelectric properties of organometallic molecular junctions*. V. Delmas, S. Rigaut, V. Diaz-Cabanes, C. van Dyck, D. Vuillaume, E. Scheer, J. Cornil, and K. Costuas, in preparation.

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

Poster

The role of antiaromaticity in the single molecule conductance of dibenzopentalene compounds

Lydia Abellan,[a] Maximilian Schmidt,[b] Daniel Wassy,[b] Mathias Hermann,[b] M. Teresa González,[a] Nicolás Agräit, [a,c] Linda A. Zotti, [d] Birgit Esser [b,e,f] and Edmund Leary.[a]

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Abstract:

We will present a room temperature STM break junction study of the single molecule conductance of several novel antiaromatic compounds containing a dibenzopentalene (DBP) unit.[1] The aim of the study is to determine the effect upon the electrical conductance of replacing an aromatic group for a comparable antiaromatic unit. The compounds are based on the well-studied oligo(phenylene ethynylene) backbone with PhSMe anchor groups and we have investigated three different central units: phenyl, anthracene (both aromatic) and DBP (antiaromatic). Our results show that while the molecules with anthracene and DBP are more conductive compared to the phenyl analogue, there is little detectable difference between the former two, which is despite the DBP having the smallest HOMO-LUMO gap thanks to partial antiaromatic charachter. Theoretical calculations reveal that the reason for this is that the Fermi level lies close to the centre of the HOMO-LUMO in both cases where the difference in transmission curves is small. As the LUMO of the DBP compound is, however, lower than the other two compounds, we hypothesise that tuning the Fermi level alignment with appropriate anchor groups could maximise the difference.

References:

1. Maximilian Schmidt et al. *Chem. Commun.*, 2021, 57, 745-748

Poster

Mechanical manipulation of spin states in an all-organic di-radical molecules

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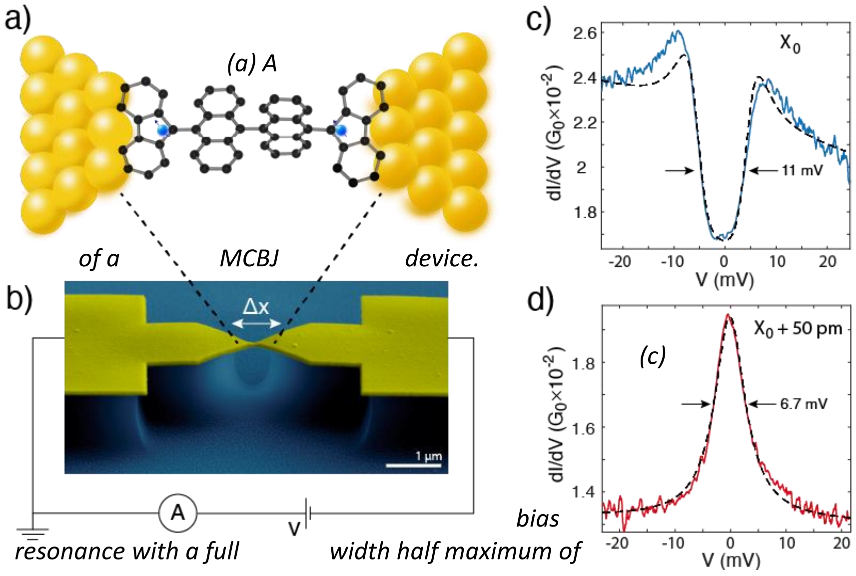
During the last years, atomically precise synthesis of poly-aromatic hydrocarbons (PAH) has been developed [1-2] for a new generation of devices using spin polarization as information carrier, storage and processing [3]. We report on mechanical manipulation of spin-spin interactions for a PAH di-radical molecule (Figure a) in a mechanically controlled break junction (MCBJ; Figure b) at low temperature. Zero-bias peaks in differential conductance spectra (Figure d) are attributed to a Kondo resonance arising from hybridization of one of the radical electrons with the metallic electrodes. Varying the distance between the electrodes affects the coupling strength leading to a spin-flip inelastic electron tunnelling spectroscopy (IETS) signal [4] in the dI/dV spectra (Figure c). Thus, by mechanical manipulation the spin signature can be adjusted and controlled. This study provides new insight on the interplay between two manifestation of magnetism in molecular-electronics.



(a) A schematic illustration of the di-radical 2-0S molecule junction with the two spins indicated by the blue spheres. (b) Scanning electron microscopy picture of a MCBJ device. Molecular features from dI/dV spectra at two different electrode positions: (c) A dip with a flat region around zero-bias produced by an inelastic spin flip excitation (IETS) and (d) a peak centered around zero-bias ascribed to a Kondo resonance with a full width half maximum of 6.7meV.

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Poster

Indirect Spin-Readout of Rare-Earth-Based Single-Molecule Magnet with Scanning Tunneling Microscopy

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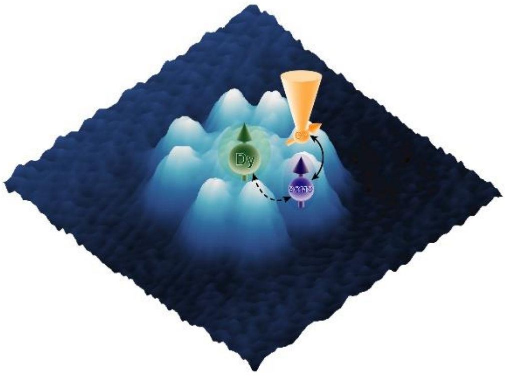
Abstract:

Rare-earth based single-molecule magnets are promising candidates for magnetic information storage including qubits as their large magnetic moments are carried by localized 4 f electrons. This shielding from the environment in turn hampers a direct electronic access to the magnetic moment. Here, we present the indirect readout of the Dy moment in Bis(phthalocyaninato)dysprosium (DyPc2) molecules on Au(111) using milli-Kelvin scanning tunneling microscopy. Because of an unpaired electron on the exposed Pc ligand, the molecules show a Kondo resonance that is, however, split by the ferromagnetic exchange interaction between the unpaired electron and the Dy angular momentum. Using spin-polarized scanning tunneling spectroscopy, we read out the Dy magnetic moment as a function of the applied magnetic field, exploiting the spin polarization of the exchange-split Kondo state [1].



Basic idea to access the Dy magnetic moment.

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Poster

Quantum Interference in Graphene-Based Single-Molecule Devices

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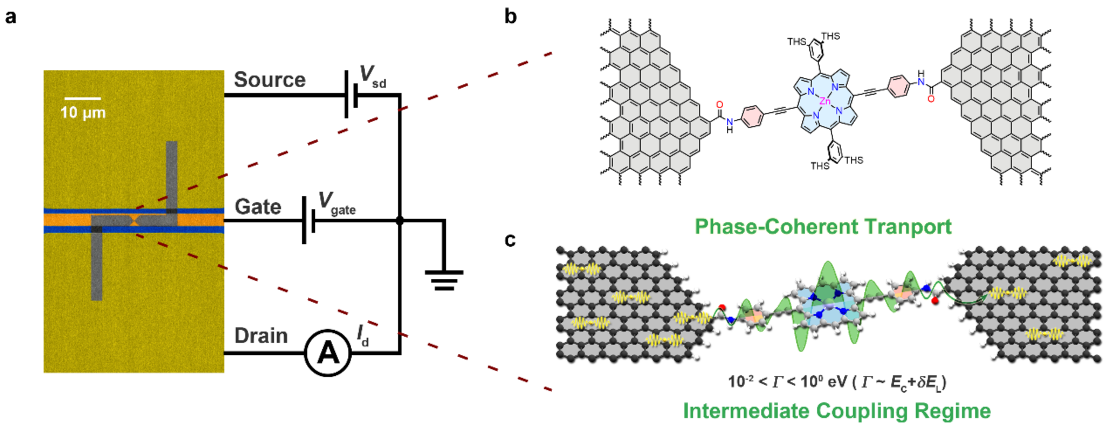
Abstract:

Quantum interference effects could either suppress or enhance charge transport through single-molecule junctions. Efficient tuning of charge transport through single-molecule devices could be achieved by controlling quantum interference. However, direct evidence for quantum interference in charge transport through single-molecule junctions have not yet been demonstrated. In our research, instead of common three dimensional bulky gold electrodes used in break junction technique, we use two dimensional graphene electrodes, for which screening effect from electrodes can be minimized and efficient gating for both molecule and electrodes can be achieved by electrostatics gate. Periodic interfering pattern for graphene were observed, magnetic field dependent behaviours were further measured, which originate from tuning the phases of electrons by bias voltage, gate voltage and magnetic field, providing the direct evidence for coherent transport through the whole single-molecule device. Antiresonance signal was found in gate dependent conductance measurement, which further demonstrates destructive quantum interference. Our findings provide direct evidence for quantum interference in charge transport through graphene-based single-molecule junctions, which is the foundation stone for the future development of quantum interference based single-molecule electronic devices.



a *False colour SEM image with the schematic representation of the electronic circuit of our device architecture. The local gold gate electrode is under a layer of HfO2 (10 nm thick).* ***b*** *Schematic display fully conjugated amide coupling molecular junction in graphene nanogap with a porphyrin core.* ***c*** *Schematic representation of phase-coherent transport process in intermediate coupling regime.*

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Poster

Fused Porphyrin Oligomers for Single-Molecule Electronics

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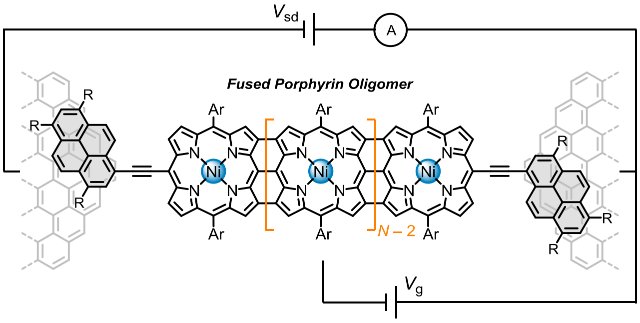
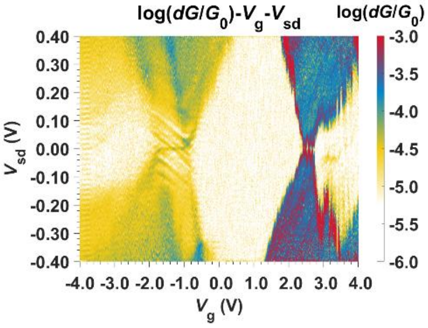
Abstract:

Conjugated porphyrin molecular wires with strongly coupled π orbitals can be used for investigating and controlling long-range charge transport properties, and are expected to be promising candidates for fabrication of electronic devices.[1] Among the porphyrin oligomers, the triply linked (edge-fused) porphyrin tapes show fascinating electronic properties and the HOMO–LUMO gap decreases steeply with length.[2] This makes porphyrin tapes exciting candidates for charge transport studies on single molecule-based devices. Despite their promising properties, there have only been reports of charge transport studies in molecules up to a fused porphyrin trimer (~ 4 nm).[3-5] Here, new advances in the synthesis and characterization of porphyrin tapes with molecular lengths up to 15 nm are presented. Studying the transport properties of such long, fully conjugated π-systems structures will allow for fundamental insights into the mechanisms and limits of molecular transport and delocalization. In addition to synthetic pathways, charge transport results from single-molecule graphene-based junctions are presented, where intermediate electronic coupling between the molecule and graphene electrodes leads to the observations of coherent transport through the junctions and Kondo resonances in their *N* – 1 charge states.





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Poster

Influence of electronic environment on molecular light emission

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Abstract:

Scanning tunnelling microscopy (STM) in combination with a light collection setup proved to be an ideal technique in order to control and understand the light emitting processes on the scale of a single molecule. In this work, based on three variants of naphthalene diimide (NDI) complexes, we use a low temperature STM with a novel light collection system [1] to induce and to control molecular light emission. We use tailor-made molecular complexes with a tripodal platform that is supposed to decouple the attached NDI chromophore from the underlying gold substrate in order to avoid quenching of the molecule's excited state by the metal's electrons. While this strategy did not work as intended and most molecules lie flat on the metal substrate, we found two ways to still sufficiently decouple the chromophore and to observe molecular light emission. First, molecular clusters that consist of multilayers of NDI molecules of unknown orientation or of standing molecules do show light emission of molecular origin with sharp peaks in the range from 1.5 eV to 2.05 eV with surprisingly high quantum yields of 1×10^{-4} to 1×10^{-3} photons emitted per tunnelling electron [2]. Second, by modifying the molecular configuration of the flat lying NDI molecules with the STM tip, it is possible to controllably drive individual molecules into a metastable state, in which they are electronically decoupled from the metal substrate. Some of these molecules show well-defined optical emission spectra with sharp emission lines, including vibrational side bands. Quantum chemical calculations allow us to assign the spectral lines to the cationic dimer of the NDI complex. Light emission from self-decoupled molecules which can be directly adsorbed on a metal substrate, opens up a pathway to study a wide range of chromophores for the further development of highly efficient and tunable emitters.

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Poster

Substitution Pattern Controlled Quantum Interference in [2.2]Paracyclophane-Based Single-Molecule Junctions

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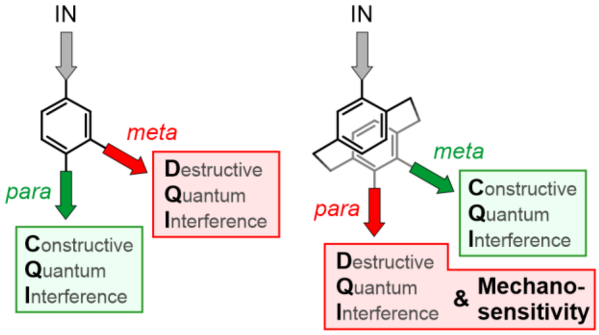
Abstract:

Quantum interference (QI) within a single-molecule junction has become an essential yet powerful concept to integrate for designing molecular electronic devices.[1] Recently we have investigated the correlation between substitution pattern, conductance and mechanosensitivity in [2.2]paracyclophane(PCP)-based single-molecule junction via the mechanically controlled break junction technique (MCBJ).[2,3] We study the influence on conductance when we introduce meta/para connection to the PCP core and the phenyl ring attached to the anchoring group. We find that (i) meta-phenyl-anchored PCP yields such low conductance levels that molecular features cannot be resolved; (ii) para-phenyl-coupled anchoring generally gives higher conductance levels which can be detected via MCBJ; (iii) pseudo-para-coupled PCP core manifests large mechanosensitivity while (iv) pseudo-meta-coupled PCP core show the absence of mechanosensitivity. These experimental findings are interpreted in terms of QI effects between molecular frontier orbitals by theoretical calculations based on density functional theory and the Landauer formalism.



Concept illustration of the substitution controlled QI

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Poster

The CISS effect: A Magnetoresistance Through Inelastic Scattering

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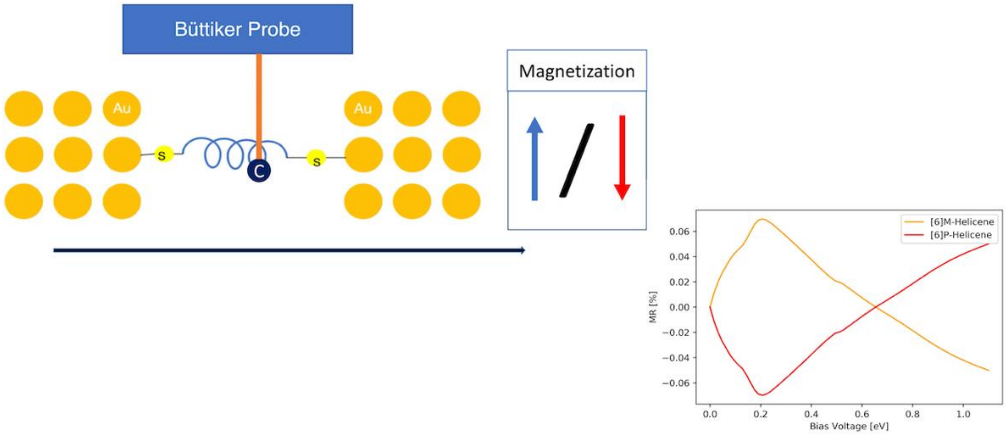
Abstract:

One of the manifestations of chirality-induced spin selectivity (CISS) is the magnetoresistance in two-terminal transport measurements on molecular junctions (1,2). This paper investigates the effect of spin-orbit coupling in the leads on the polarization of the transmission. A helicene molecule between two gold contacts is studied using a tight binding model. In order to study the occurrence of magnetoresistance, which is prohibited in coherent transport, as a consequence Büttiker reciprocity (3), we add Büttiker probes to the system in order to incorporate inelastic scattering effects. We show that for a strict two-terminal system without inelastic scattering the magnetoresistance is strictly zero in the linear and nonlinear regimes. We show that for a two-terminal system with inelastic scattering, a nonzero magnetoresistance does appear in the nonlinear regime, reaching values of the order of 0.1%. Our calculations show that for a two-terminal system respecting time-reversal symmetry and charge conservation, a nonzero magnetoresistance can only be obtained through inelastic scattering. However, spin-orbit coupling in the leads in combination with inelastic scattering modelled with the Büttiker probe method cannot explain the magnitude of the magnetoresistance measured in experiments.



Schematic picture of the gold-sulfur-helicene junction. A Büttiker probe is attached to a carbon atom of the helicene molecule. The magnetoresistance for this junction is calculated for [6]M-helicene and [6]P-helicene and it is plotted on the right as a function of bias voltage.

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Poster

Quantum Interference in Radical and Neutral Single-Molecule Junctions

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Abstract:

Quantum interference (QI) in single-molecule junctions creates an anti-resonance in the transmission function near the Fermi energy which usually translates in a decrease of the conductance (*G*) and in an increase of the Seebeck coefficient (*S*) (1). In particular, this phenomenon appears in molecules with *meta* connections (2). Here we present an experimental study of the *G* and *S* in single molecules by comparing *para*- and *meta*-connected fluorene derivatives (2) and Blatter radicals (3) using a scanning tunneling microscope (STM) at room temperature and ambient conditions. Our results reveal the importance of the intrinsic spin state of radicals for a simultaneous enhancement of *G* and *S* and the influence of QI in these transport properties.

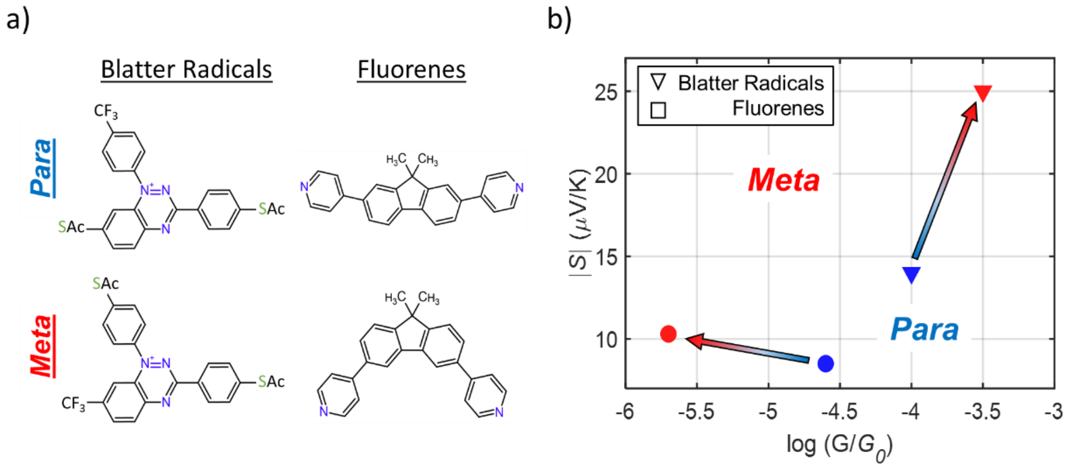

Figure 1: ***a)*** *Scheme of the compounds investigated,* para- *and* meta- *connected Blatter radicals (left) and fluorenes (right).* ***b)*** *Seebeck coefficient (S) vs conductance (G) values for* para- *(blue) and* meta-connected *(red) Blatter radicals (triangles) and fluorenes (circles). The arrows highlight the effect of QI on the transport properties when the connection changes from* para *to* meta*.*

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10th International Conference on Molecular Electronics
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Poster

Isocyanides: strong anchoring groups for gold electrodes.

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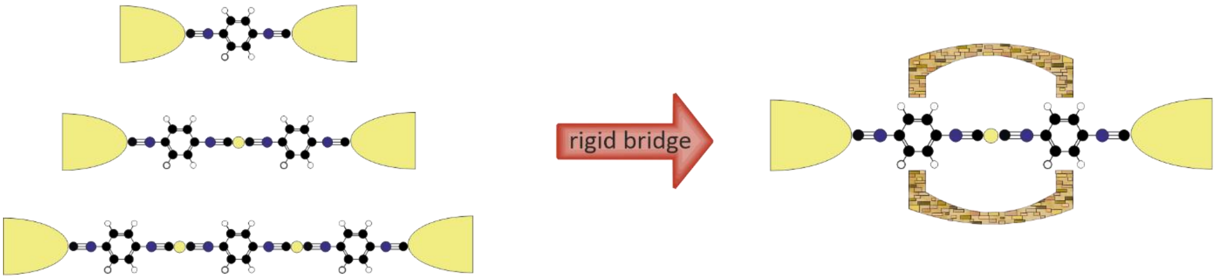
Abstract:

The increasing complexity of molecular electronics, in particular the high tunable structure-property relation and the mechanical modulation of single molecular junctions set high requirements to the anchoring groups necessary in these studies. These include a high affinity to the electrode, an effective orbital hybridization and a matching Fermi energy level. Furthermore, high junction formation probabilities are of advantage and required for possible applications.

The most common and studied anchoring group for single molecular electronics with gold electrodes is the thiol, forming a strong coordination bond which still allows sliding. Recent studies suggest, that isocyanides to gold interaction is stronger than the thiol one.[1] In particular Tysoe *et al.* showed, that when 1,4-diisocyanide is deposited on an Au(111) surface, Au-CN bonds are immediately formed.[2] Furthermore, isocyanides seem to possess a higher surface mobility while showing more stable I-V curves than thiols.[3] The finding of Calame *et al.*, showing a 99% junction formation probability as well as the formation of a one dimensional oligomer when increasing the electrode displacement in a MCBJ setup subject to a 1,4-diisocyanide solution.[4] This suggests, that the isocyanide to gold interaction is stronger than the gold to gold one.

To further study the isocyanide to gold interaction we decided to bridge two 1,4-diisocyanide units to investigate the junction formation probability, conductivity as well as the affinity of the system to gold. Furthermore, favored bidentate complexation with gold can be studies.



Bridging of two 1,4-diisocyanide units for the investigation of macrocyclic systems with isocyanide anchoring groups in mechanically controlled break junctions.

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Poster

Engineering the transport orbital in a molecular junction

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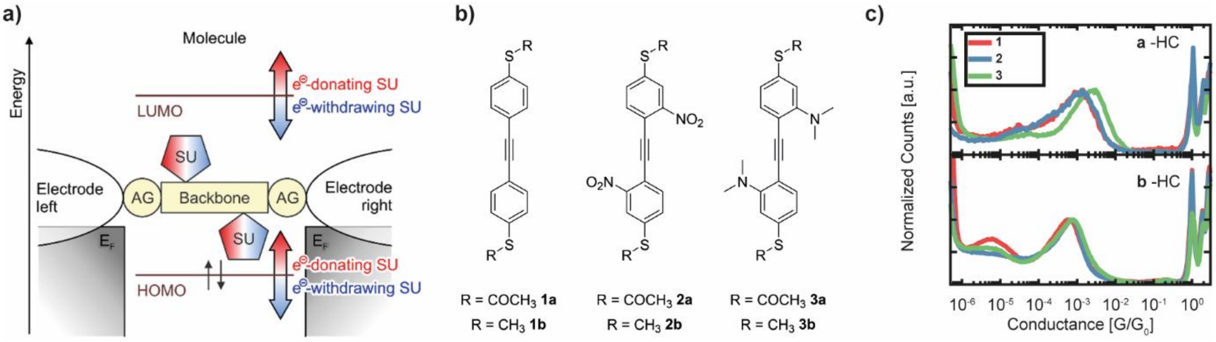
** authors with equal contribution*

Abstract:

Metal-molecule-metal junctions are of fundamental interest for integration in electronic devices as molecules are the smallest objects whose properties can be tailored by chemical design[1]. Tuning charge transport through molecules requires engineering of the molecular orbital whose energy lie closest to the Fermi level of the contacts. This can be achieved through the introduction of proper side-groups on the molecular backbone[2]. In this work we study the charge transport properties of a series of tolanes using the Mechanically Controllable Break Junction (MCBJ) technique, paired with Density Functional Theory (DFT) calculations. The molecules have been substituted either with electron-withdrawing nitro-groups, or electron-donating dimethylamino-groups. Effects of the anchoring were also investigated by using two different types of binding groups: thioacetate- and methylsulfanyl-, which form covalent and dative bonds to gold respectively. The investigated side groups are able to shift the energy levels and shrink the HOMO-LUMO gap as expected, as shown both by DFT calculations, Cyclic Voltammetry and UV/Vis spectroscopy. However, MCBJ measurements do not reflect these changes. This effect can be explained with DFT calculations by considering that the Fermi energy of the contacts can take on a wide range of values.



a) Scketch of the molecular junction where the molecule is linked to the electrode by anchor groups (AG), and its energy levels are tuned by substituents (SU). b) Chemical structure of the investigated molecules. c) Conductance histograms of the high-conductance plateau found in the MCBJ measurements.

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Poster

Three-state molecular potentiometer based on a non-symmetrically positioned in-backbone linker

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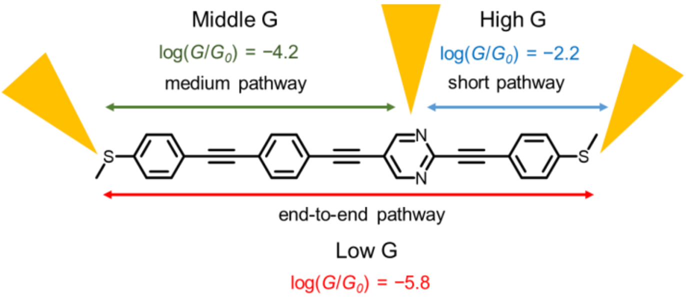
Abstract:

The examples of molecular potentiometers, in other words regulable resistors, are scarce.[1,2] In this direction, molecules presenting multiple conductance values as result of the co-existance of different conduction pathways along the molecular backbone are highly promising. Here, we report on the synthesis and single-molecule conductance of a *para*-oligo(phenylene)ethynylene (*p*-OPE) derivative with three well-defined conductance states. Employing theoretical models and comparing to reference compounds we show that this effect is due to the nonsymmetric positioning of a pyrimidine ring, acting as an in-backbone anchor group, which opens up two new additional conduction channels.[3] This strategic system displays three conduction pathways which differ distinctively in both conductance and length. In this way, the conductance value could be modulated by selecting an electrode distance for the molecular junction that suits with the appropiate pathway.



The pyrimidine-based p-OPE prepared is able to give rise to three well differentiated conductance values due to distinguishable conduction channels along the molecular backbone.

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Poster

Electrode effects on the observability of destructive quantum interference in single-molecule junctions

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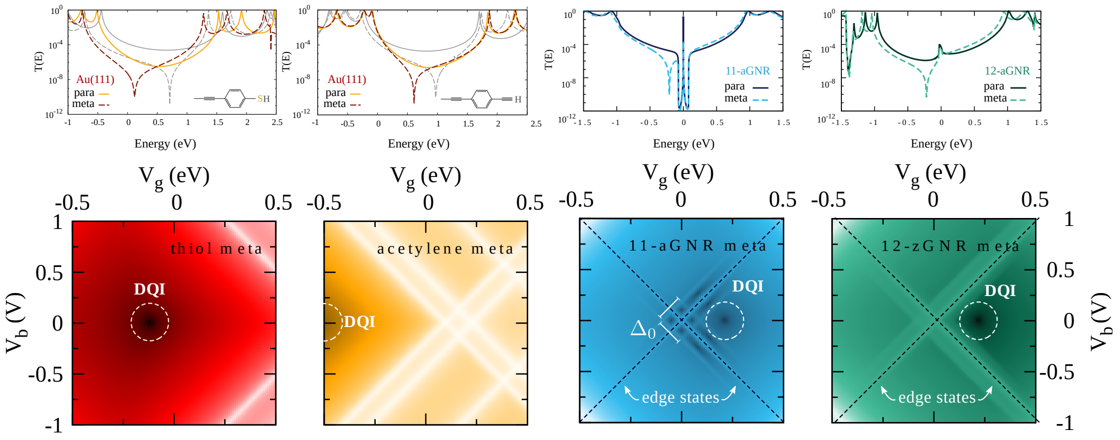
Abstract:

Destructive quantum interference (QI) has been a source of interest as a new paradigm for molecular electronics as the electronic conductance is widely dependent on the occurrence or absence of destructive QI effects. In order to interpret experimentally observed transmission features, it is necessary to understand the role played by all components of the junction, including the molecular core, the linkers, and the electrodes. First principle calculations allow assessing the structure-function relation for quantum transport through pyrene molecular junctions with distinct QI properties, and to capture a complexity that is beyond simple Hückel model calculations. A thorough analysis allows to disentangle the transmission features arising from the molecule and the electrodes and determine the observability of destructive QI. We also suggest that QI can be relevant for chemical sensing. The adsorption of small gaseous molecules (NO_2, H_2O, and NH_3) on pyrene is systematically investigated varying the adsorption site and adsorbate orientation in order to understand the selectivity properties of graphene-like junctions. Our study can potentially be useful for developing graphene-based sensors exploiting QI effects.



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Poster

Mechanically controlled destructive quantum interference in naphthalene based paracyclophanes

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Destructive quantum interference is known to be present in certain paracyclophane (PCP) type structures [1,2], which can be mechanically controlled as mechanical deformations cause a change in the frontier molecular orbital arrangement around the Fermi energy. Here, we present a study on a naphthalene based PCP containing a backbone of stacked naphthalene groups with on both sides a connection to a thiol group for anchoring to the gold electrodes. Using the mechanically controlled break junction technique the single-molecule conductance is investigated at room temperature. To explore the mechanosensitivity of the single-molecule junction, we perform electrode displacement modulation experiments, where the conductance of the single-molecule junction is monitored as the electrode displacement changes in a periodic fashion. We observe three different mechanosensitive behaviors: in-phase, antiphase and double frequency. The double frequency response can be directly attributed to the presence of destructive quantum interference. As an outlook we show the ability to study the temperature dependence of this behavior.

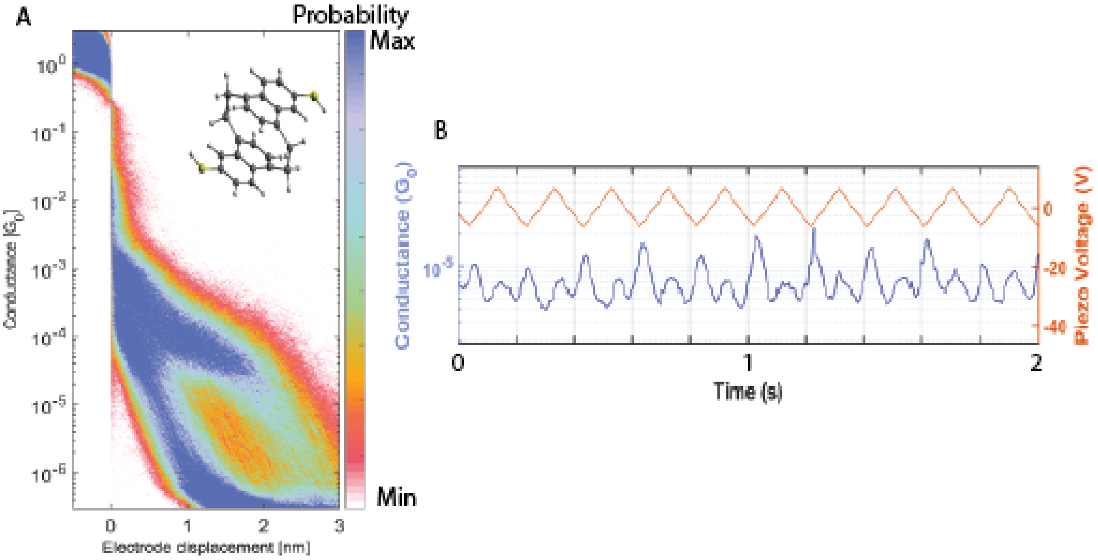

Figure 1: A) Conductance vs. distance density plot, with in the inset a schematic of the molecule. B) Electrode displacement modulation experiment with in blue the conductance and in red the piezovoltage that is used to modulate the electrode displacement. The conductance displays double the frequency compared to the modulation, indicating that the transmission through the molecule traverses the quantum interference dip while being modulated [1,2].

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Towards Electron-triggered Coordination-induced Spin State Switching in Viologen-based Metal Complexes

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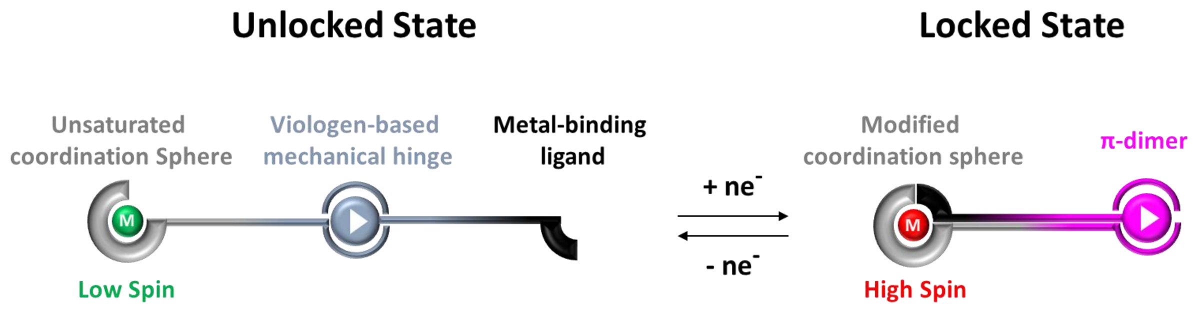
The control of magnetic properties by external stimuli has attracted much interest over the past few decades and tremendous work has been achieved thereafter.[1] Our contribution to this field is based on the **C**oordination-**i**nduced **S**pin **S**tate **S**witching approach (***CiSSS***)[2] which, as its name implies, aims at changing the spin state of a metal center by modifying its coordination sphere. Therefore, based on our expertise in supramolecular chemistry and with the help of theoretical calculations, a well-suited model system was designed and eventually synthesized. In this presentation, the targeted tweezer-like molecule features a redox-responsive viologen-based hinge tethering a high affinity ligand to a magnetically active metal center. In agreement with the concept depicted below, the electrical stimulation of the hinge is expected to trigger a large amplitude molecular motion driven by the reversible, intramolecular π-dimerization of the electrochemically-generated viologen cation radicals.[3,4] This fully reversible back and forth self-locking process will enable to control the coordination/dissociation of the ligand to/from the metal center and, consequently, its spin state. The spin-state switching process will be discussed on the grounds of spectroscopic, electrochemical and spectro-electrochemical data supported by quantum calculations.



Electron-triggered self-locking behaviour for reversible CiSSS.

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Poster

Plasmon-Induced Grafting in the Gap of Gold Nanoparticle Dimers for Plasmonic Molecular Junctions

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Abstract:

Gold nanoparticle (NP) dimers of various shapes have been fabricated on ITO by e-beam lithography. The gap separating two NPs was set to 30-50 nm. Oligo(bisthienylthiophene) was then grafted onto these substrates by plasmon-induced diazonium salt reduction (1,2). We show that this organic semi-conductor can be selectively grafted onto these NPs and that growth is strongly affected by light polarization. When light is polarized in the direction perpendicular to the dimer axis, a 15 nm-thick layer of oligo(bisthienylthiophene) is observed on each NP with minimal grafting between them. On the contrary, when light is polarized in the direction of the dimer axis, oligomer deposition occurs mainly between the gold NPs and completely fills the 30-50 nm gap. As a consequence, plasmonic molecular junctions are obtained in a few minutes in a massively parallel process (3,4).

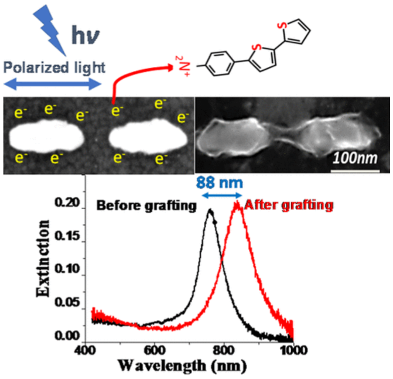

Figure : Schematic illustration of the strategy for plasmon-induced grafting onto dimers under polarized light; SEM image of NR dimers after oligo(BTB) plasmoninduced grafting using polarized light along X and Extinction spectra of gold NR dimers before and after oligomer grafting

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Poster

Molecular mechanisms involved in organic-based non-volatile memories elucidated through the use of a multiplex platform.

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Characterization and comprehension of molecular mechanisms involved in organic-based non-volatile memories remains an important key to their development.[1] Multiplexed platform (**MP**) fabrication is a promising way to explore layers properties in different ways, combining different complementary techniques such as AFM, XPS, Raman *in-situ*, and I-V characteristics.[2] Here we propose to develop multiplexed devices (Figure 1) with organic actives layer come from electroreduction of diazonium organometallic salts.

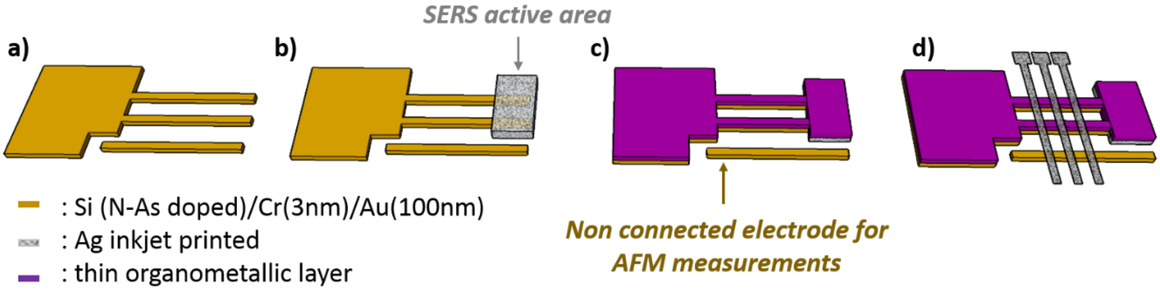

Figure 1: Schematic illustration of the fabrication of the multiplex platform. a) photolithography of the gold bottom electrode electrode, b) silver pad printing, c) electrografting of the organometallic layer, d) top silver electrode printing.

To build the **MPs**, gold electrodes are first made by photolithography onto silicon. A silver pad is then deposited onto these electrodes by ink-jet printing to form a rough conductive surface that presents a SERS effect. This allows to analyze the Raman signature of the active organic layers that are then further deposited electrochemically.[3] Moreover, a homemade cell was designed to perform SERS measurements under electrochemical conditions. Finally, silver top electrodes are ink-jet printed on the molecular film to allow memory addressing and I-V curves recording. The non-connected electrode serves as a reference for AFM measurements.

Preliminary results show that our films exhibit diode behavior and that there is no short-circuit, showing that the devices are well elaborated regarding molecular deposition and electrode printing. On NABD films, the irreversible reduction of nitro group and the open/close azo bound were observed both by CV and on the Raman mapping. Further complementary investigations (AFM, Raman in the solid state combined to I-V characteristics, XPS) are underway to complete the description and will be also presented.

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Poster

Organic Switching Devices processed from Water-Soluble Conductive Polymer and their Characteristics

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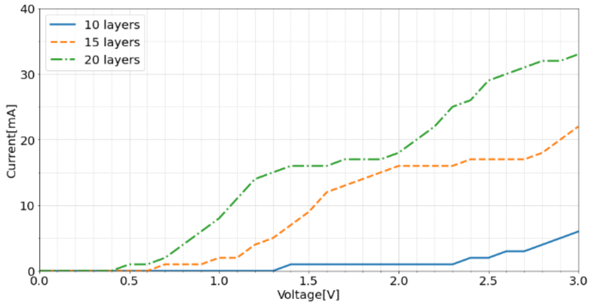
Abstract:

We observed a quantum step-wise current of ca.1.6 mA (pro 0.8-2V) on a thin film of a water-soluble conductive polymer. Water soluble conductive polymer is new material synthesized by Japanese chemical company TOSO and we use it as a collaboration. It is difficult to laminate a thin and uniform film of water-soluble conductive polymer on a highly water-repellent material. We laminate such thin film on plastic substrate by spraying fine mists repeatedly. After each spraying, we quickly dried the solvent water of the mist and get fine particles of the conductive polymer molecules. Then we measured the electronic spectroscopy of the two-dimensional electromagnetic field, i.e., the DC V-I characteristics of the thin film of conductive polymers as we stacked them layer by layer. Step-wise increasing structure of current with periodicity of 0.16mA was observed in all the samples[Fig.1]. ON-SET voltage decreases from 1.3 V to 0.5 V as the number of spraying increased from 10 to 20 times. We continuously repeated this process from 10 to 70 times and observed the ON-SET voltage gradually decreasing and drawing close to the asymptote of bulk V-I linear characteristics formed by conventional application of macroscopic solution[Fig.2]. No current was observed under the ON-SET voltage, and beyond the threshold stable current is observed. This shows a possible device of ORGANIC SWITCHING SEMICONDUCTOR. The authors show best thanks to TOSO Co. for their providing newly synthesized material.



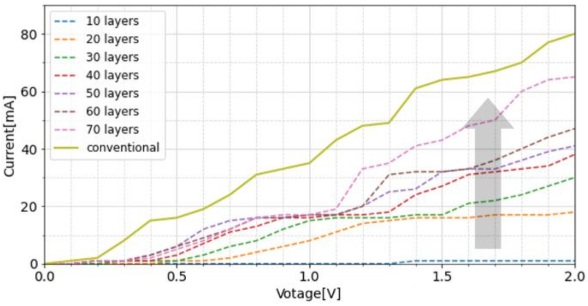


Fig.1 Quantum step current with 0.16mA in the electron spectroscopy of self-doped PEDOT thin film.(left)

Fig.2 Changes in V-I characteristics according to the numbers of accumulated layers(right)

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Poster

Large-area self-assembled gold nanoparticle superlattices for plasmonic and memory devices

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Abstract:

Self-assembled monolayer gold nanoparticles provide a convenient platform for studying electronic and optical properties of molecular junctions. Meanwhile, various structures and devices with sub-wavelength dimensions have been achieved due to strong light-matter interactions around their surface plasmon resonance frequencies [1,2]. Especially, ordered structures with (sub-)nanometer plasmonic gaps are desirable for intensive electromagnetic field enhancement, efficient quantum energy transport, and strong coupling effects [1-3]. Yet fabrication of large-area (~cm²) self-assembled gold nanoparticles with high degree of order, and (sub-)nanometer plasmonic gaps remains challenging [4,5]. In this work, we demonstrated self-assembled monolayer gold nanoparticle superlattices having areas larger than 1 cm², which were produced by an evaporation driven process at the liquid-air interface. The diameters of monodispersed gold nanoparticles are beyond 10 nm, and these particles are capped by either oleylamine or alkanethiol ligands. The as-obtained superlattices possess hexagonal symmetry, where single domains with size exceeding 10*10 µm² were observed. Via *in situ* ligand exchange, the interparticle media and separations in the superlattices can be actively tuned, leading to significant variations in their plasmonic resonance behavior. Furthermore, direct patterning of the self-assembled gold nanoparticles using E-beam lithography, followed by an emulsion-based development process, allowed us to produce compact devices with footprint from few tens to hundreds of nanometers [6]. Accordingly, we demonstrate compact memristive devices featuring experimentally verified changes in conductivity up to three orders of magnitude for set currents in the range of nA.

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Poster

Formation of organic bi-layers by stepwise electrochemical reduction of diazonium compounds: Bottom-Up Approach

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This work describes an electrochemical bottom-up approach for modification of metallic electrode to modulate the electrochemical properties of the layer. The adopted strategy is based on two successive electroreductions of diazonium salt and was successfully used in the fabrication of molecular junction with specific behavior.[1] The deposited ultrathin layers consist of an electron donating oligo (bisthienylbenzene) (BTB) and an electron acceptor namely oligo (phenyl methylbipyridium) (PMV^{2+}). The generated bilayers are studied by AFM, XPS, XPS depth analysis and electrochemical techniques. The study demonstrates the possibility to graft one layer over the initial one to create strongly coupled donor-acceptor or acceptor-donor bilayer systems with minimal interpenetration and overall thicknesses between 5 and 20 nm. The electron transfer towards redox probe in solution and electron transfer in solid state molecular junctions are studied.[2,3] The electrochemical response of several outer-sphere redox probes on such modified electrodes is close to that of a diode, thanks to the easily p-doped oligo (BTB) or easily reducible oligo (PMV) moieties. Moreover, the electron transport in solid state molecular junctions exhibits strong rectification with opposite sign depending on the order of the two layers. Our goal in this work was to control the electronic response through the structuration and the functionality of the organic layer.

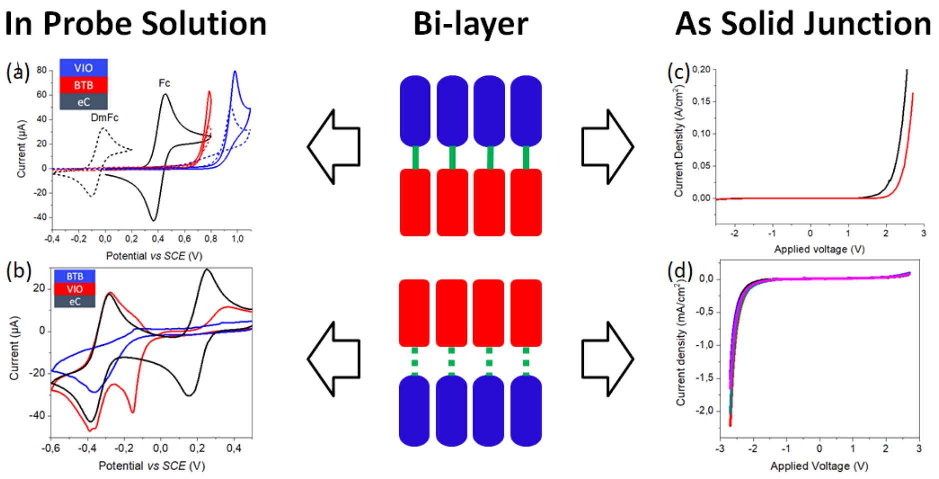

Figure 1: CVs of bare (black curve), single layer modified electrode (red curve) and bilayer modified electrode (blue curve) in Fc solution (5mM), DmFc(5mM) (a) and TCNQ(5mM)(b). Scan rate 100 mV.s^{-1}; *JV* curves for Au/BTB/PMV/Ti(c) and Au/PMV/BTB/Ti (d) junctions.

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Poster

Graphene-organic semiconductor structures for vertical organic transistors

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Abstract:

The great advantage of vertical organic transistors consists in having a much shorter channel lengths and higher switching speeds than planar thin film transistors [1]. The organic permeable base transistors architecture is very promising to create complementary circuits operating in the MHz range [2][3]. Strategies to push the transistor performances in the GHz frequency range have already been presented [4].

In this context, we investigate the vertical charge transport and the injection mechanisms at the graphene/organic semiconductor interfaces. By incorporating graphene as a semi permeable base into the transistors architecture, we seek to improve the control over the electro statics of the device, and to enable the fabrication of flexible electronic devices operating at low-voltage and high frequency. In this preliminary study, we show the structural and electrical properties of vertical hetero-structures composed of graphene and C60.

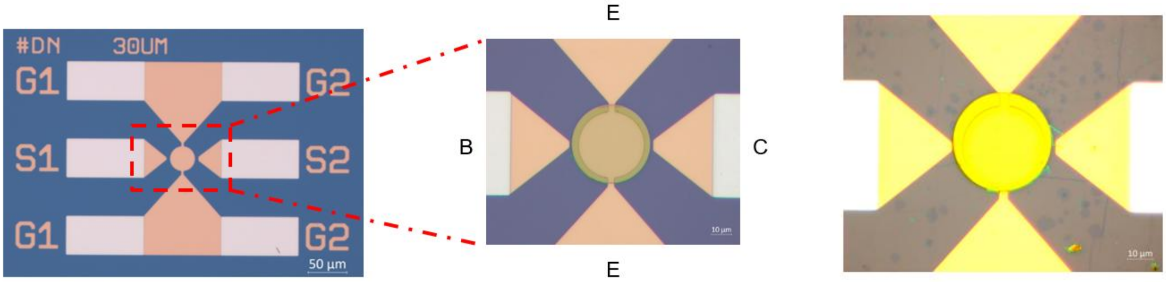

Figure 1: Left) Optical microscope image of the Au/C60 vertical stack. Right) Enhanced optical microscope image showing the graphene electrode on top of C60.

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Poster

Reversible temperature-induced switching in Spin Crossover thin film tunnel junctions.

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Abstract:

Spin Crossover (SCO) complexes are a family of materials displaying two stable electronic configurations, that can be reversibly tuned using appropriate stimuli (temperature, pressure, light irradiation, magnetic field etc…). It has been predicted – but shown only in a handful of cases – that the conductance of spin-crossover tunnel junctions could be altered by switching their spin state, which makes them targets of high interest for the development of switchable molecular devices. Measuring such devices is highly challenging, due to the fragile nature of the spin transition involved (both in terms of stability of the molecules and of robustness of the SCO process to external constraints), which has limited the number of successful experimental studies demonstrating this effect so far. We will present a complete study ranging from the preparation of high-quality continuous thin films of spin crossover complexes of Fe(II) with scorpionate ligands families, their characterization, and the experimental and theoretical study of the electrical properties of metal-insulator-metal tunnel junctions, in which the SCO complexes constitute the switchable molecular insulator [1-2]. We will present ultra-thin switchable spin crossover vertical tunnel junctions in which the spin-state switching of the films – due to reversible temperature-driven spin crossover – persists at the nanoscale, and induces an abrupt change in the tunnelling current density flowing through the junction. Those results on large-area junctions demonstrate the high potential of SCO-based switchable molecular junctions as functional devices.

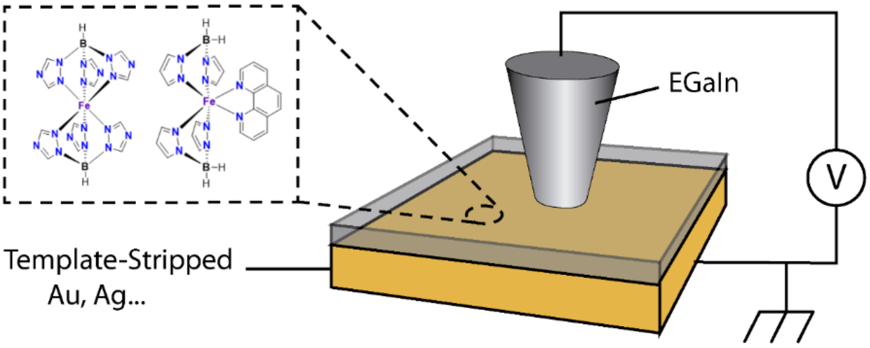

Figure 1: Representation of an SCO thin film vertical tunnel junction. A thin film of spin crossover complexes (see inset on the left) is deposited on a conductive substrate, and the transport properties are probed using an EGaIn electrode.

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Poster

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

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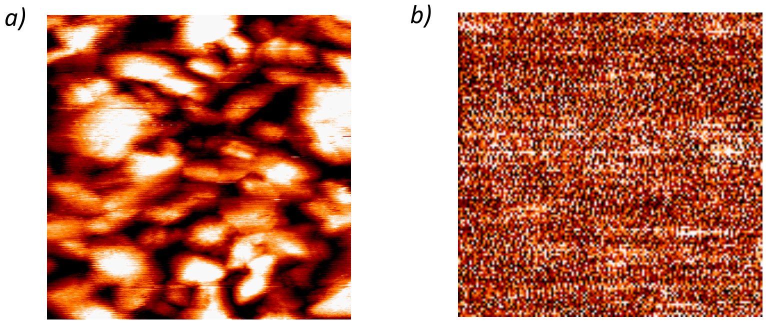
Abstract:

In the field of spintronics, there are many reasons to use molecular tunnel barriers in devices such as low cost, flexibility and long spin lifetime in organic materials [1,2]. What happens at the interfaces in these organic-inorganic hybrid systems is so relevant to the properties that a word has been proposed for it: spinterface [3]. The discrete nature of 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 (spin valve). 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) and X-ray photoelectron spectroscopy (XPS). To avoid the formation of pinholes during deposition of the Co ferromagnetic top electrode of the spin-valve, 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 magneto-transport properties of these model 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 Co(3nm)/C16MT/GaAs(001), 100x100nm^2, U_{gap}=2.4V, I_t=15nA. The homogeneity of the BEEM current map demonstrates the absence of pinholes.

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Poster

Switching polyoxometalate monolayers by light irradiation

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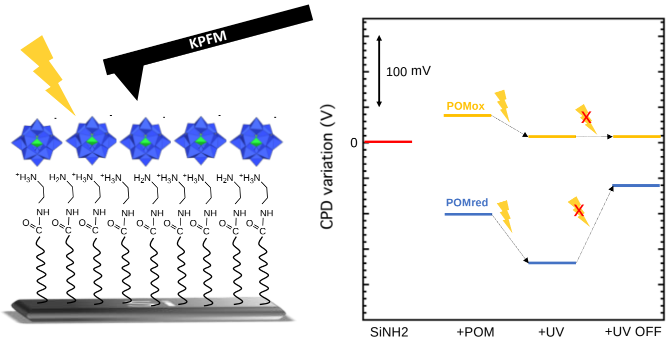
Polyoxometalates (POMs), nanometric oxo-clusters made of early transition metals in their highest oxidation state, are promising molecules with remarkable physical properties, and are at the heart of intense research work to integrate them into molecular-based materials and molecular-based devices.[1] Especially, they can be switched from one stable state to another thanks to various stimuli (electric field, light irradiation, magnetic field…), making them good candidates to play the role of molecular memories.[2] More precisely, some of them are photoreducible, which means that it is possible to switch the molecule from its oxidized state to its reduced states by UV-irradiation.[3] Whereas the photoreducibility of polyoxometalates has been widely studied in the bulk state or in multilayers, it has never been studied at the nanometric scale, i.e. at the monolayer or single-molecule level.[3-4] In this presentation, the first evidence of the photoreduction of a monolayer of POMs will be presented. The Keggin-type polyoxomolybdates $(n\text{-}Bu_4N)_3[PMo_{12}O_{40}]$ and the corresponding one-electron reduced species were electrostatically deposited onto a NH_2/NH_3^+-terminated organic self-assembled monolayer on silicon. Emphasis was given on the surface characterization and on the understanding of the immobilized POM photoreduction properties using especially the non-intrusive KPFM technique to follow the variation of the redox state of the POM's layer under in-situ UV-irradiation.



(left) General scheme of the KPFM measurements of a monolayer of $[PMo_{12}O_{40}]^{3-}$ under UV irradiation (right) variation of the contact potential difference at the surface with or without UV irradiation

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Poster

Investigation of carbazole based compounds as electroactive materials for organic electronics

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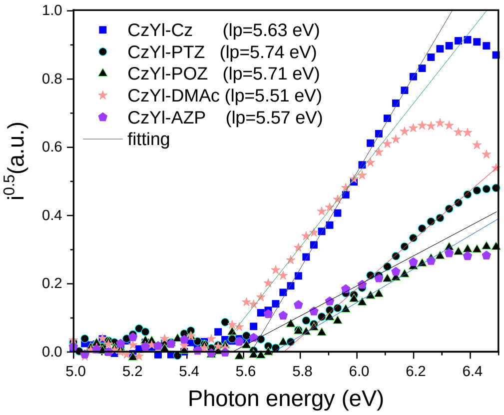
Abstract:

Recently, a great deal of attention was given to organic hole-transporting materials in organic electronics. These materials play a crucial role in injection and transporting of holes in organic devices [i]. It is well established that carbazole based materials exhibit good hole-transporting properties [ii]. In our work we synthesized and investigated the photo physical properties of a new series of carbazole based compounds. The solid amorphous state for the materials is highly appreciated due to their ability to form homogeneous films in the organic devices [iii]. The materials displayed thermal stability with weight loss temperatures higher than 300°C. Their glass transition temperatures ranged from 63˚C to 104˚C. The photoluminescence quantum yields ranged from 1 to 22% for deoxygenated toluene solution and from 0 to 5% for neat films. Photophysical measurements revealed that the singlet-triplet energy splitting values ranged from 0.34 to 0.59 eV. The materials exhibited hole drift mobilities reaching 10^{-3} $cm^2/(Vs)$ at high electric fields and displayed relatively high ionization potentials ranging from 5.5 eV to 5.7 eV. Taking into account the measured parameters, these compounds are regarded as promising candidates for hosts or hole transporting materials for OLEDs and other optoelectronic devices.



Electron photoemission spectra

Acknowledgement

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Poster

Novel hole transporting materials pyrazolopyrimidine and imidazopyrimidine derivatives for perovskite solar cells

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Abstract:

Perovskite solar cells (PSCs) have attracted much attention due to various advantages, such as simple solution processing, low manufacturing cost, and high performances. The high performance of PSCs (up to 25% power conversion efficiency in 2020[1]) is related to the electronic and energetic properties of the perovskite active layer such as widely tunable band gap, high absorption coefficient, high charge mobility, long carrier lifetime, and long charge diffusion lengths [2]. However, the hole transporting material (HTM) layer used in these devices play an important role in their efficiency and stability [3]. To date, **Spiro-OMeTAD** is still the most efficient HTM in PSCs, which has been widely investigated due to good solubility in organic solvents, suitable energy levels and a limited absorption in the visible light region [4]. However, the synthesis of Spiro-OMeTAD is relatively complicated due to harsh synthetic conditions, such as multiple steps and aggressive or sensitive reagents[5]. For these reasons, several alternative HTMs based on carbazole derivatives [6,7,8] have been developed in our group, gather simplier synthesis and efficiency in PSCs.

In this communication, we present our recent work on the development of new HTMs based on a **pyrazolopyrimidine (A)** or **imidazopyrimidine (B)** core. The chemistry allows functionalization of these core with one, two or three **4,4'-dimethoxydiphenylamine 3,6-disubstituted carbazole (C)** moieties (Fig.1). Their physico-chemical properties such as electronic, energetic and thermal properties have been measured to assess their potential in PSCs. Then, these molecules have been used as HTMs in PSC devices (**$FTO/SnO_2/FA_{0.85}Cs_{0.15}Pb(I_{0.85}Br_{0.15})_3/HTM/Au$**) and their PV properties have been evaluated, compared with **Spiro-OMeTAD** based devices. A study of the relation structure/properties have been guided, particularly in function of the chemical structure of the core and the number/position of grafted carbazole moieties (**C**).

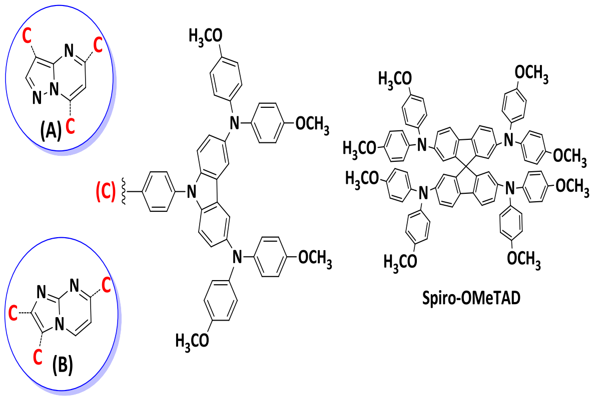

Figure 1 :Chemical structure of HTMs studied

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Poster

New host materials for high performance blue single layer phosphorescent light emitting diodes

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Abstract:

Nowadays, OLEDs (Organic Light-Emitting Diodes) technology is present in everyday life. It is mainly found in smartphone and television screens, but also, more recently, for lighting. Organic electrophosphorescent diodes (PhOLEDs) are the second and most mature generation of OLEDs. In this technology, all the high-efficiency PhOLEDs are multi-layer devices constituted, in addition to the emissive layer (EML), of a stack of functional organic layers. These layers play a crucial role in the device performance as they improve the injection, transport, and recombination of charges within the EML. However, in order to fit with the energetic and ecological transition, PhOLED technology should still be improved. Single-layer PhOLEDs (SL-PhOLEDs) represent ideal OLEDs, consisting only of the electrodes and the EML[1]. Simplifying the multilayers structure is then crucial to reduce the amount of commodities, the manufacture complexity, the production and recycling costs for real-life applications. However, reaching high-performance SL-PhOLED is far from easy, as removing the functional layers of an OLED stack dramatically decreases the performance. To achieve high SL-PhOLED efficiency, the efficient injection, transport, and recombination of charges should be insured by the EML, and particularly, by the host material[2-4]. Herein, two host materials have been investigated. They are constructed on the association of an electron-rich unit (indoloacridine or dihydroquinolinoacridine) connected by a shared spiro carbon atom to an electron-deficient 2,7-bis(diphenylphosphineoxide)-fluorene. In addition to a high E_T value, adequate highest occupied molecular orbital/lowest unoccupied molecular orbital energy levels and important thermal stability, the key point in this molecular design is the suitable balance between hole and electron mobilities, which leads to good performance in a SL-PhOLED. In this work, the synthesis and the study of photophysical, electrochemical and charges transfer properties are reported and rationalized by theoretical calculations. Then, the performances of the SL-PhOLEDs using these semi-conductors as host materials are presented.

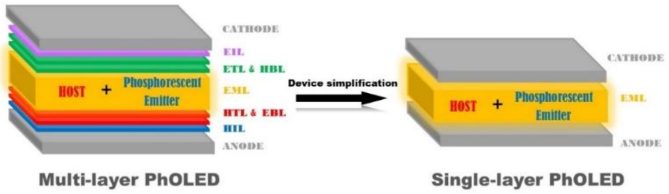

Figure. Schematic representation of a multi-layer PhOLED (left) and a single-layer PhOLED (right).

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Poster

Matched Rectenna Design Using Organic doped diode for Textile Integration

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Abstract:

There is a growing demand for remotely controlled and powered wireless devices such as in remote sensing and health monitoring applications where the use of wires or exchanging batteries may not be feasible. Additionally, the ambient wireless power density is on the rise due to an exponential growth in electromagnetic power sources like mobile base stations, Wi-Fi routers and TV. Hence, there is an increased interest in radio frequency (RF) energy harvesting using rectennas. Rectennas which are used to convert electromagnetic energy into electric energy are characterised by very high losses partly steeming from the diode. However, the use of organic diode despite only feasible for low power applications and at low frequencies can help minimize the losses.

We use organic diode from pentacene and P3HT in designing rectenna for operation at 13.56 MHZ. However, the rectenna would need to be integrated into a circuit on textile for its desired application and the performance is largely determined by the efficiency of the antenna to capture sufficient energy and the rectification efficiency of the diode to convert the energy. Since different impedances that lead to reflection and inefficiency define the antenna and diode, the design of the matching circuit to match the output impedance of the antenna to the input impedance of the diode was critical and more so because of the integration into textile. The Advanced Design System (ADS) simulation software was used for the simulations because of the RF tools available for designing matching circuits and evaluating efficiency of the rectifier circuit.

In the simulation, passive circuit (inductors and capacitors) was used in designing the matching circuit since it can be replicated on the textile. The result for a load of 5kΩ shows that the pentacene diode rectenna has a maximum efficiency of 21% for an input power of 2dBm while with the P3HT diode, it was 57% for -2dBm input power. Furthermore, using the voltage doubler configuration of the diode with two diodes, the maximum efficiency for the pentacene diode became 15 % at its peak for an input power of 2dBm with the output voltage becomes 1.6 V from 1.2 V of using a single diode. Similarly for voltage doubler configuration of P3HT diode with two diodes, the maximum efficiency is 47% for 4dBm input power and the output voltage increased to 2.6 V from 1.6 V. The obtained results provide the first step for the design of the rectenna with an organic doped diode for textile integration.

This work was supported by European Project Interreg Luminoptex and ANR Context project.

Poster

Optoelectronics properties of some new tetracyclic azaheterocyles

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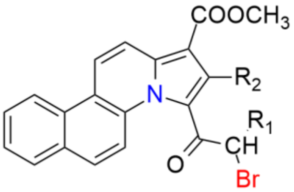
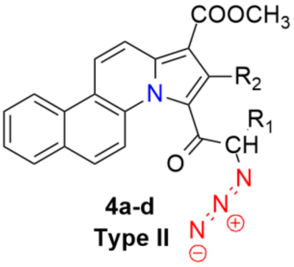
Abstract:

During the last decades azaheterocyclic derivatives, and particularly tetracyclic azaheterocyles, are reported as highly valuable materials in medicine and pharmacy (drugs, as antibicrobial, anti-HIV, anticancer, analgesic, antidepressant, antihypertensive, anticoagulants, etc.), agriculture (mainly herbicides and grow up factors), optoelectronics (fluorescent and electroluminescent materials, semiconductor devices, sensors and biosensors), etc. This is why, obtaining of such derivatives continues to generate interest from large research teams from academia, industry, agriculture.

Tetracyclic azaheterocyles are 18 π-electron *N*-fused heterocycle, containing a bridgehead nitrogen atom shared by an electron-excessive pyrrole and an azine electron deficient six-membered ring, and represent a very interesting class of compounds for optoelectronic applications, most of them being pure blue emitting derivatives. As part of our ongoing research in the field optoelectronic properties of azaheterocyclic derivatives, we present herein our results concerning the synthesis and opticalspectral properties of two new classes of tetracyclic azaheterocyles (Type I- 3-(bromoacetyl)benzo[f]pyrrolo[1,2-a] quinolone and Type II- 3-(azidopropanoyl)benzo[f]pyrrolo[1,2-a]quinolone) which can be used as fluorescent building blocks for optoelectronic applications.



2a-d
Type I



4a-d
Type II

The tetracyclic azaheterocyles were synthesized by a straight and efficient metod: heterogeneous catalysis bromination of previously obtained azaheterocycles derivatives, followed by the nucleophilic substitution of the bromide with azide group. The synthesis was performed both under conventional thermal heating and under ultrasound (US) irradiation. Under US irradiation the yields were substantially higher, the reaction time decrease dramatically (from days to hours), whereas the solvent amounts required are at least three-fold less compared to conventional heating. Taking into consideration these advantages, the proposed method should be considered environmentally friendly.

Acknowledgements. This work was supported by a grant of the Romanian Ministry of Education and Research, project number CNFIS-FDI-2021-0546.

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Poster

Chiral propeller radical based SAMs

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Abstract:

Chirality is a very important property of molecules and biomolecules but also nanoparticles. Pharmaceutic action, some smells and tastes, Life (ADN helix), etc, are governed by chirality. Synthetic materials properties and the devices properties derived from them can be modulate by chirality. In organic materials chirality can determine the optical behaviour, molecular recognition and conductivity. [1] For example, it was demonstrated by Naaman et al. the action of chiral molecules in electron spin polarized transport (Chiral induce spin selectivity-CISS).[2] Our group has deeply studied the preparation of persistent organic radicals-based materials and, in particular those derived from the Perchlorotriphenyl methyl (PTM) radical. This radical is paramagnetic, redox active, fluorescent and also chiral. [3,4] Remarkably, the circularly polarized luminescence behaviour for PTM enantiomers was recently reported. [5] Also, Interestingly, towards practical applications in devices, PTM radical has been grafted on different surfaces (silicon, gold, ITO, HOPG) via alkyl, thiol, silane and and diazonium salt groups, respectively). [6,7]

Here we present the preparation of thin-films of a PTM derivative having terminal alkyne groups able to react with gold[8]. First, PTM radical Plus (P) and Minus (M) atropisomers were separated by HPLC and characterized by Circular Dichroism (CD) in solution. The thermodynamic barrier was determine using a chromatographic method (ΔG=21.6kcal/mol). Although fast racemization was found in solution, stable thin films, of both enantiomers, could be prepared at low temperature. The CD response of the resulting films revealed high stability, showing the total racemization at 80ºC. Furthermore, thanks to the -C≡C-H functional groups self-assembled monolayers of both enantiomers were successfully prepared. Monolayers were characterized by XPS, cyclic voltammetry and RAMAN. Results reveals a good coverage of the surfaces, and a good stability of the grafting.

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Poster

Organic small molecules as a hole-transporting materials for efficient perovskite solar cells

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Nowadays hole-transporting materials (HTM) based on conductive small organic molecules and polymers have become the hottest topic in high-performance perovskite solar cells (PSCs). Over the past few years, great progresses have been made in perovskite solar cells though the investigation is still in progress [1].

Perovskite solar cells (PSCs) have been brought into sharp focus in the photovoltaic field due to their excellent performance in recent years. The power conversion efficiency (PCE) has reached to be 25.2% in state-of-the-art PSCs due to the outstanding properties of perovskite materials as well as progressive optimization of each functional layer, especially the active layer and hole transporting layer (HTL) [2]. Generally, HTL plays particular roles as following it extracts and transports the holes in the active layer to the electrode, it acts as an energy barrier to prevent the transfer of electrons to the anode, it separates the perovskite layer from the anode and isolates the moisture in the air, improving the devices stability by reducing possible degradation and it can help to improve the open circuit voltage when its highest occupied molecular orbital (HOMO) energy level is well matched[3 4].

In this presentation, synthesis and optical, electrochemical, charge-transporting properties of new inexpensive hole-transporting materials based on carbazole, dibenzofuran or dibenzothiophene cores intended for applications in organic light-emitting diodes and perovskite solar cell will be reported.

The presented information can be helpful in developing stable and effective PSCs. The results presented in this contribution will give a new possibility for the design and investigate new organic HTMs for PSCs. However, we hope that the results obtained in this work can be useful for the development, synthesis and characterization of compounds that can be used in the development of organic light-emitting diodes and organic photovoltaic cells.

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Acknowledgement:
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Poster

Micro-Mesoporous Conjugated Polymer Based on Poly (Imides-Triazine) as a High-Performance Organic Li-Ion Battery Cathode

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Abstract:

Organic electrode materials have gained great attention owing to their capability to reach high capacities, their tunable structures and their versatility and sustainability.[1] However, the solubility of those compounds into organic electrolytes, their mid-range potential and the poor electronic conductivities of non-conjugated organic materials have limited their further application.[2]

In this context, Covalent Organic Frameworks (COFs) provide an opportunity to take organic electrodes to another level. These porous polymer generated upon covalent assembly of organic monomers are attractive structures for Li-Ion batteries cathodes with extended lifetime and higher energy storage capabilities due to their high capacity/mass ratio.[3] Unlike traditional organic polymeric materials, COFs have robust framework structures with high versatility, porosity and stabilities.[4]

Poly(Imide-Triazine) (PIT) material was previously synthesized and detailed as gas storage and biomolecules adsorption.[5,6] In this work, we reported a new application of (PIT) as covalent organic framework cathode materials for Lithium-ion Batteries (LiBs). Compared with previously described PIT, our material exhibited a high specific BET surface area of 647,26 $m^2.g^{-1}$ and a hierarchically porous structure to trigger interfacial Li storage and contribute to an additional capacity. Electrochemical studies reveals that after an activation process, the synthesized cathode delivered a reversible specific capacity about 310 $mAh.g^{-1}$ at 0.5 $A.g^{-1}$, an excellent rate behavior (260 $mAh.g^{-1}$ at 5 $A.g^{-1}$) and a good cycling stability over 1000 cycles at 6 $A.g^{-1}$, involving that the developed polymer cathode afford a promising organic electrode for high-performances and durable energy storage devices.

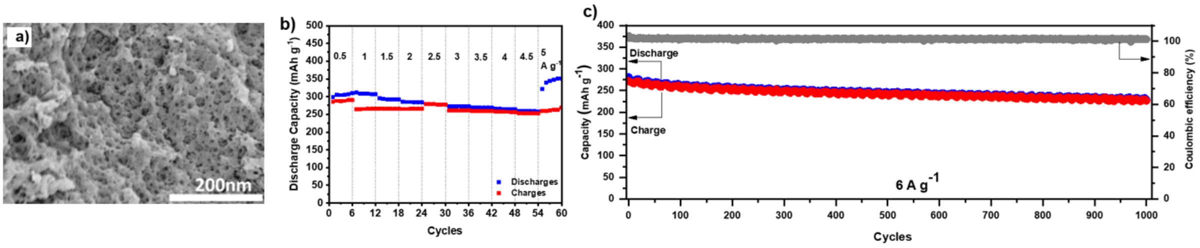

Figure: (a) The SEM image of PIT, (b) rate capabilities at different current densities, and (c) cycling performance at 6 $A.g^{-1}$

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Poster

Organic doped diode rectifier based on Parylene-electronic beam lithogrpahy process for Radio frequency applications

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Abstract:

We have adapted a "peel-off" process to structure stacked organic semiconductors (conducting polymers or small molecules) and metal layers for diode microfabrication. The fabricated devices are organic diode rectifier in a coplanar waveguide structure. Unlike conventional lithographic process, this technique does not lead to destroy organic active layers since it does not involve harsh developer or any non-orthogonal solvent that alter the functionality of subsequentially deposited materials.

This process also involves recently reported materials, as a p-dopant of an organometallic electron-acceptor Copper(II) trifluoromethanesulfonate, that play the role of hole injection layer in order to enhance the performances of the diode.

Comparatively to self-assembled monolayers based optimized structures, the fabricated diodes show higher reproducibility and stability. High rectification ratio for realized pentacene and poly(3-hexylthiophene) diodes up to 10^6 has been achieved. Their high frequency response has been evaluated by performing theoretical simulations. The results predict operating frequencies of 200 MHz and 50 MHz for pentacene and P3HT diode rectifiers respectively, with an input oscillating voltage of 2 V peak-to-peak, promising for RFID device applications or for GSM band energy harvesting in low-cost IoT objects.

This work was supported by European Project Interreg Luminoptex and ANR Context project.
We thank the French National Nanofabrication Network RENATECH for financial support of the IEMN Cleanroom.

References:

Organic doped diode rectifier based on Parylene-electronic beam lithogrpahy process for Radio frequency applications; K. Ferchichi, S. Pecqueur, D. Guerin, R. Bourguiga, K. Lmimouni; *Organic Electronics* 97 (2021) 106266

Poster

Untangling the electronic and charge transport properties of new Naphthalene and Perylene Diimides based-semiconductors.

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Abstract:

Organic semiconductors have emerged as an important class of materials that offer interesting prospects for high throughput, low-cost and flexible electronic circuits. Nevertheless, high-performance electron-transporting (n-type) semiconductors are still rare compared to their high efficiency hole-transporting (p-type) counterparts. In this sense, the development of high-mobility and environmentally stable n-type materials for thin-film transistors has experienced a tremendous impetus in the last decade. Naphthalene-diimides (NDIs), perylene-diimides (PDIs) and their derivatives have demonstrated great potential as n-type semiconductors in Organic Field-Effect Transistors (OFETs).[1-3] In this project, a mixed experimental and theoretical study of four new semiconductors (Figure 1) has been carried out with the aim to explore the impact of the following effects on the electronic and charge-transport properties: (i) the extension of the conjugated platform, going from a shorter conjugated core in naphthalene-diimides to a larger conjugated core in perylene-diimides, (ii) the different donor units attached to the cores. For that, IR, UV-Vis absorption spectroscopy, and spectroelectrochemical measurements have been used in combination with theoretical calculations based on the Density Functional Theory (DFT). In addition, the four studied compounds have been implemented in OFETs , to assess their potential as active materials in organic electronics.

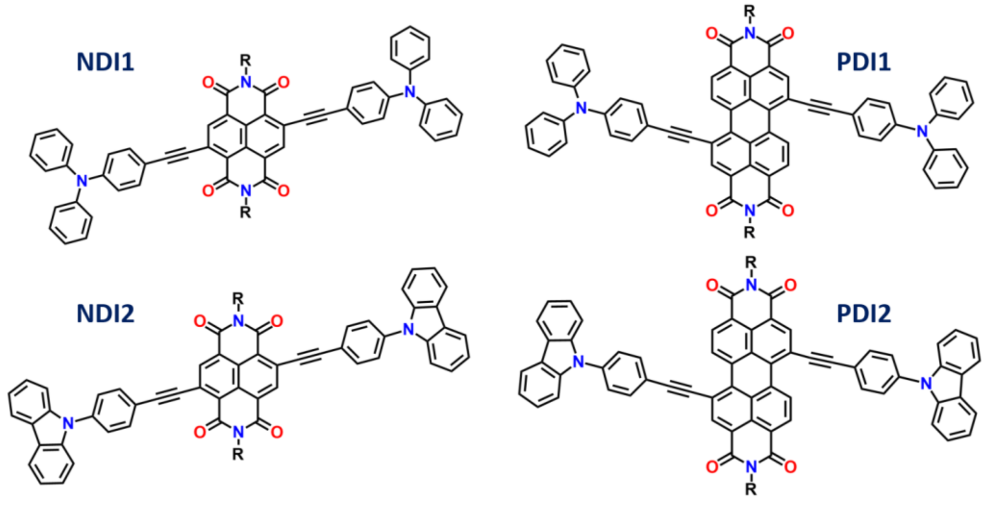

Figure 1. Chemical structures of NDI and PDI compounds under study.

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Poster

Prototyping a fully textile rectifier circuit operating at 13.56 MHz

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Abstract:

The recent rise of smart textile brought a multitude of new flexible connected devices [1]. However, they aim to be wearable and the power supply questions stay problematic. A way to resolve this issue is to use electromagnetic field, especially the near field communication to transfer energy and data from wearable sources, for example the mobile phone, to the different sensors embedded into our garment. Textile NFC antennas and combiners have already been developed [2], they can receive a 13.56 MHz magnetic field. This work focuses on the development of a textile rectifier circuit. It has been designed by ADS to operate at 13.56 MHz. Every current line in the final prototype is composed of 3 overlapped conductive yarns "Datatrans" from Tibtech company. The capacity pF, has been realised by two 300 mm parallel current lines. The inductance is composed of a 6 turns and 80 mm outer diameter coil. The capacity pF, is composed by a four branches of 150 mm interdigitated current lines. Even if the embroidery process enables to create electric component, it only enables making one line pattern. Consequently, the final prototype is a superposition of several patterns that are connected by soldering to insure the current continuity. Finally, both 1N4148 commercial diode and P3HT organic rectifier has been soldered into the dedicated spot. First results show that there is a 300 mV continuous signal when the circuit is power supply by a 13.56 MHz and 2V signal.

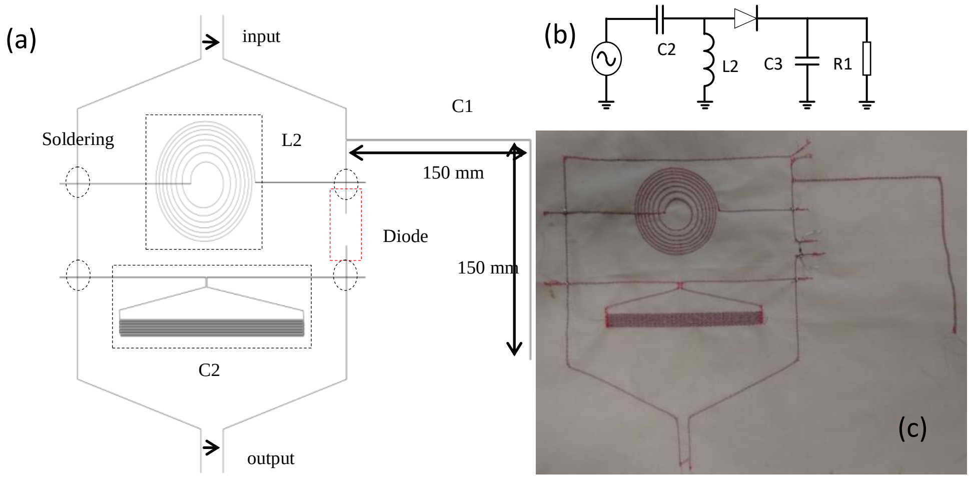

Figure 1. Textile rectifier circuit (a) embroidery and (b) electrical diagram. (c) Photography of the prototype

This work was supported by European Project Interreg Luminoptex and ANR Context project.

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

Long-lived CPL active chirality-at-rhenium complexes bearing a helicenic NHC ligand: structure-properties relationships to enhance chiroptical & photophysical performances.

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Helicenes are made of *n ortho*-fused aromatic or heteroaromatic rings. This helical structure thus formed can furnish inherent chirality and remarkable properties such as high optical rotation values (in comparison with chiral pool compounds). Helicenes were used as molecules displaying strong chiroptical properties and as enantioselective ligands in asymmetric catalysis, to name a few.[1] On the other hand, N-Heterocyclic Carbenes (NHCs) are a well-defined class of electron-rich ligands with a versatile design, known to form strong metal-carbene bonds in organometallic complexes.[2] Recently, by combining these 2 chemistries, our group has been able to prepare iridium complexes with enantiopure helical carbene ligands which display long-lived light-green circularly polarized phosphorescence.[3] Following these results, we have interested ourselves on the design of helicenic N-2-pyridyl-NHCs and their use as chiral ancillary ligands in transition metal complexes. We have achieved the synthesis of rhenium (I) complexes (**1**) which possess helical chirality (P/M) and less common chirality-at-rhenium (A_{Re}/C_{Re}).[4] All pure stereoisomers of **1** were obtained by chiral HPLC resolution and their photophysical (absorption, emission) and chiroptical properties (optical rotation, circular dichroism and circularly polarized luminescence) were examined. Complexes **1** exhibit long-lived green circularly polarized phosphorescence. Interestingly, we have observed that the stereochemistry & the nature of the halide ligand bonded on the rhenium (I) center give rise to strong differences regarding polarized & unpolarized emission properties, helping to the fine optimization of the performances (Fig 1.).

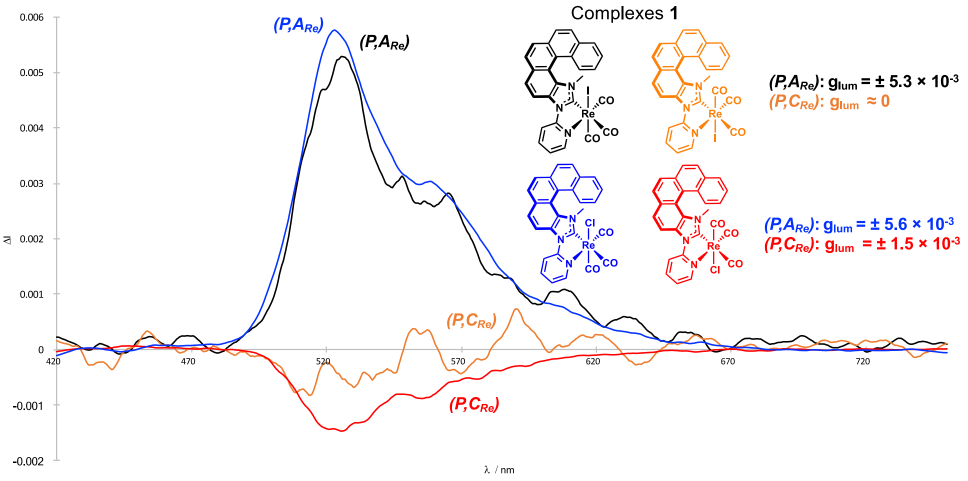

Fig 1. CPL spectra of enantiomeric pairs of **1** *measured in degassed CH_2Cl_2 at r.t.*

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Poster

Multichromophore Systems for Entropy-Driven Singlet Fission

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Abstract:

Solar energy has the highest theoretical potential of all renewable energy sources. Despite the enormous development in the last few decades, all single-junction solar cells share fundamental loss mechanisms that limit their theoretical efficiency to 33%. Singlet fission (SF) is a process where a singlet exciton formed by the absorption of one photon can evolve into two triplet excitons, hence, increasing the thermodynamic limit of solar cells to 45%. In the last decade, significant effort has been made to improve understanding of SF mechanism and structure-property relationship. The core building blocks for these studies were pentacenes, which triplets have energies around 0.8 eV. However, the application of SF in silicon-based solar cells requires high-energy charge carriers (above 1.1 eV). Such high-energy triplets, derived from SF, are accessible by thermal or entropic activation of endothermal singlet fission.[1]

Our interest in multichromophoric molecular systems lies in the development of a scalable model for entropy-activated singlet fission. This talk will give an overview of our efforts towards chromophore assembly, ranging from covalent binding to complexation around metal centers; theoretical and experimental studies of the entropy-activated endothermal SF; and structure-property relationship resulting from the above that will be valuable tool for the design of an ultimate SF photovoltaic material.

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

Poster

Direct arylation of push-pull triarylamine dyes based on difluoro-benzothiadiazole units and their evaluation as active material for OPVs

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Abstract:

Two push-pull molecules involving a triarylamine donor unit connected to a dicyanovinyl acceptor moiety by a difluorobenzothiadiazole-thienyl block have been synthesized. In order to simplify the synthesis, avoid intermediate halogenation reactions and the formation of toxic organometallic by-products, building blocks were connected by direct (hetero)-arylation.[1,2] The optimization of the experimental conditions of the coupling reactions was studied as well as the preliminary evaluation of the potential of the target compounds as active material in simple air-processed organic solar cells.

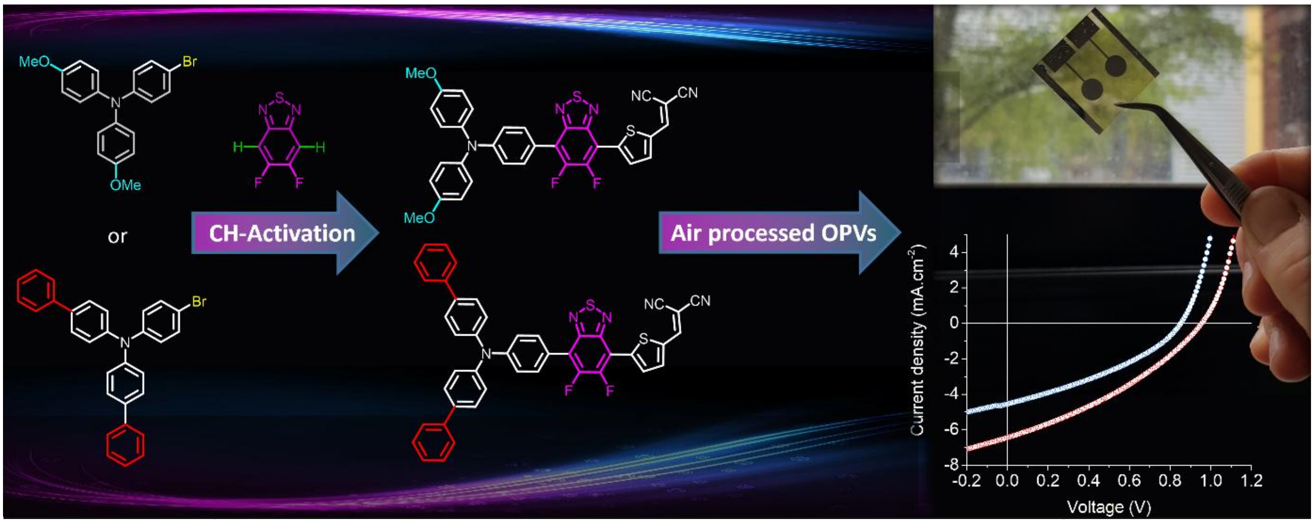

Figure: *Structure of the two push-pull molecules and the current density–voltage characteristics of the best* ***MD-OMe*** *(blue) and* ***MD-Ph*** *(red) based organic solar cells.*

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Poster

Investigation on organic thin-film transistors by Kelvin Probe Force Microscopy (KPFM)

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Abstract:

A KPFM experiment has been developed to perform surface potential measurements on operating transistors in ambient air [1]. Applied to the characterization of contact resistances in organic thin-film transistors (TFTs), the method makes it possible to separately measure the intrinsic I-V characteristics of the source and drain contacts, regardless of whether the contacts have linear or non-linear characteristics. In this work, the measurements are performed on air-stable p-channel organic TFTs [2,3], some of which exhibit linear contact characteristics and others non-linear contact characteristics (Figure 1). Results will be discussed.

Additionally, the external phase feedback loop [1] allows continuous measurement of the oscillation phase shift versus tip voltage parabola, linked to the capacitance of the AFM tip / air / charge carrier system (Figure 2). The opening of the parabola is highly sensitive to the distance between the AFM tip apex and the charge carriers, allowing one to observe the variation of the charge location depth along the transistor channel, from the source to the drain, and depending on the TFT operating condition.

Also, a method to experimentally determine the lateral resolution of the surface potential measurement will be described. The method consists of measuring the potential step on two biased electrodes separated by a narrow gap of only 12 nm. The measured profile is simulated by the convolution of an abrupt potential step with a Gaussian tip response function (Figure 3). The tip response FWHM is determined. From the measured surface potential at the source contact edge of operating transistors, extraction of the longitudinal electric field is then possible. Electric fields exceeding 400 kV.cm^{-1} have been observed on organic TFTs with non-linear contacts. This brings new insights into the charge injection process at metal/organic semiconductor contacts.

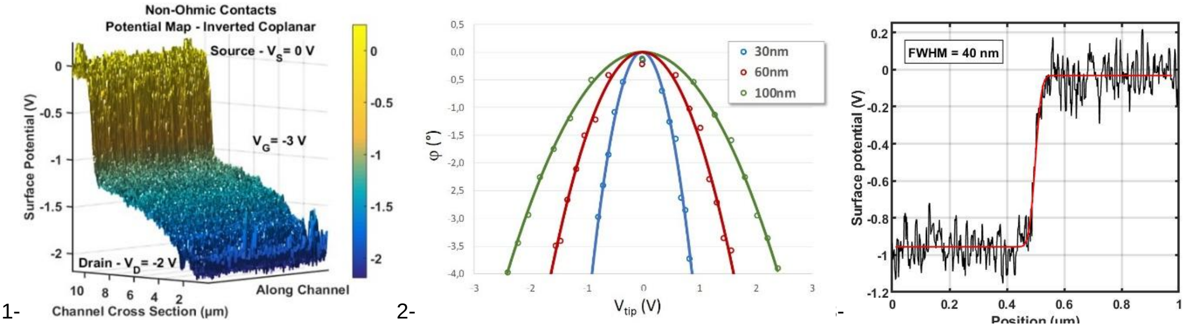

Figure : 1- Surface potential map in the channel of an organic TFT with non-linear contacts, showing strong asymmetry between the source and drain contacts. 2- Cantilever oscillation phase shift versus tip voltage for lift heights of 30 nm, 60 nm and 100 nm. 3- Potential profile measured on biased electrodes separated by a gap of 12 nm, from which the KPFM lateral resolution is determined.

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Poster

Highly fluorescent organic radical molecules arranged into nanoparticles for nanothermometry.

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[c]Networking Research Center on Bioengineering, Biomaterials and Nanomedicine (CIBER-BBN), Bellaterra, 08193, Spain

Abstract:

The tris-(2,4,6-trichlorophenyl) methyl radical (TTM) molecules present interesting optoelectronic properties [1]. These molecules are considered as inert carbon free-radical for their high chemical and thermal stability. Its open-shell molecular electronic configuration gives place to promising optoelectronic characteristics, like emission at large wavelengths, large Stokes shift or emission lifetime of the order of ns[2]. Despite such interesting properties, there are some limiting factors for nanothermometry: water compatibility, low fluorescent quantum yield or low photostability. Recently, several molecular approaches have been proposed to enhance these fundamental parameters, highlighting the development of organic nanoparticles (ONPs). Nanoparticles are very promising arrangement for organic molecules, giving them higher biocompatibility and stability in water. Here we report the preparation of organic radical NPs and their optical behavior. The NPs are made up of blends of the optically neutral tris(2,3,4,5,6-chlorophenyl)methane (TTM-αH), as a matrix, doped with the optically active TTM radical. Demonstrating that TTM radical molecules, shaped like ONPs shows a clear improvement of luminescence and photostability[3]. These ONPs exhibit a dual fluorescence emission due to radical monomers and excimers at higher wavelenghts. While the monomer emission is almost unaltered varying temperature (internal reference), the excimer emission decrease its intensity while increasing temperature (Figure). Moreover, the intensity of these emissions can be modulated with a magnetic field (18 T at 4.2 K) [4] and its excited-state dynamics has been measured using optically detected magnetic resonance (ODMR) corroborating the excimeric emission[5].

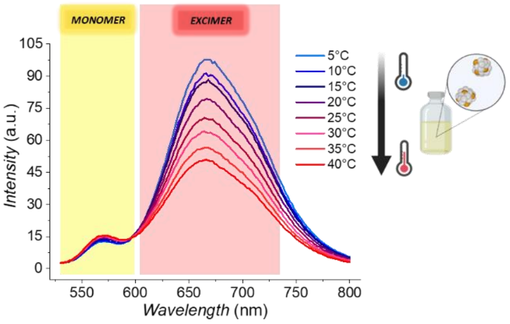

Figure : Temperature-dependant fluorescence emission spectra of TTM radical doped ONPs suspended in water.

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Poster

Electronic properties of Naphthalimide derivatives

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Abstract:

Molecular systems have proven to be efficient active materials in electronics, making then suitable substitutes of the inorganic semiconductors used nowadays in electronic devices. For this reason, organic electronics has emerged as a research field with great potential and interest. In this project we have studied, both experimentally and theoretically, two ladder-type compounds functionalized with naphthalimides[1] (Figure 1). The two molecular systems have been implemented in organic field effect transistors[2] (OFETs), to assess their potential as active materials in organic electronics. Both compounds show p-type type mobility, moreover, NDI-TP-Ph-TP material also displays low n-type mobility, presenting a certain ambipolar character. The nature and stability of the charged species involved in the charge transport process have also been studied by spectroelectrochemical experiments.

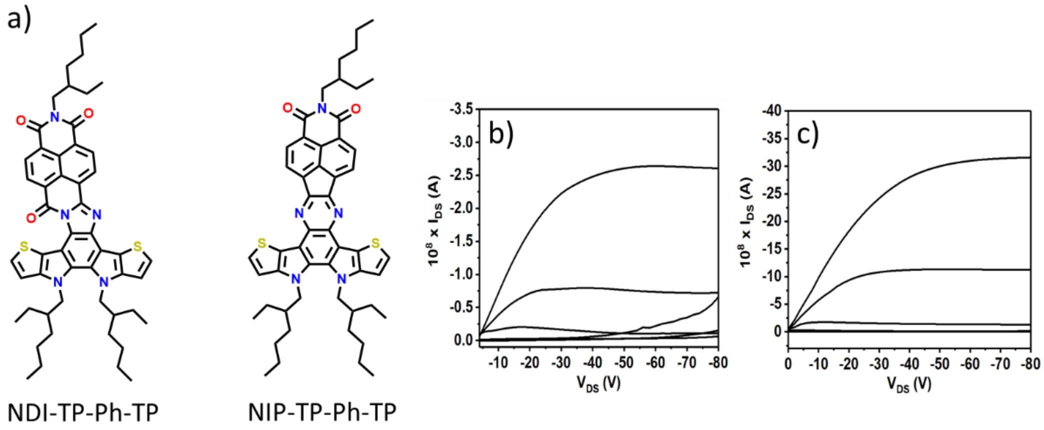

Figure 1: a) Chemical structures of the studied ladder-type systems, b) and c) OFET output curves for NDI-TP-Ph-TP and NIP-TP-Ph-TP respectively (V_{GS} ranges from 0 to 80 V in steps of 1 0V)

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Poster

Derivatives of pyrimidine-5-carbonitrile and carbazole for sky-blue OLEDs and luminescent sensors of oxygen

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Abstract:

Evolution of organic light-emitting diodes (OLEDs) reached the point, which allows to obtain maximum internal quantum efficiency of 100 % partly using heavy-metal-free emitters exhibiting thermally activated delayed fluorescence (TADF) [1]. Such emitters are also predictively perfect candidates for new generation of optical sensors since triplet harvesting can be sensitive to different analytes (at least to oxygen) [2]. Although many organic TADF emitters have been reported so far as OLED emitters, investigation of materials suitable for both OLEDs and optical sensors remains extremely rare. Aiming to achieve high photoluminescence quantum yields in solid-state and triplet harvesting abilities of organic semiconductors with efficient bipolar charge transport required for application in both blue OLEDs and optical sensors, symmetrical donor-acceptor-donor organic emitters containing pyrimidine-5-carbonitrile electron withdrawing scaffold and carbazole, *tert*-butylcarbazole and methoxy carbazole donor moieties were designed, synthesized and investigated as the main objectives of this study. The newly synthesized compounds were investigated optical and photoelectron spectroscopy, time of flight technique, electrochemistry and thermal analyses. Demonstrating advantages of the molecular design, the synthesized emitters exhibited sky-blue efficient TADF with reverse intersystem crossing rates exceeding 10^6 s^{-1}, aggregation-induced emission enhancement with photoluminescence quantum yields in solid state exceeding 50 %, hole and electron transporting properties with charge mobilities exceeding 10^{-4} $cm^2/V{\cdot}s$, glass-forming properties with glass transition temperatures reaching 177°C. Sky-blue OLEDs with non-doped light-emitting layers of the synthesized emitter showed maximum external efficiency of 12.8 % while the doped device with the same emitter exhibited maximum external efficiency of 14 %. The synthesized emitters were also used as oxygen probes for optical sensors with oxygen sensitivity estimated by the Stern-Volmer constant of 3.24×10^{-5} ppm^{-1} [3].

Acknowledgement

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Poster

Development of a correlative protocol for depth-resolved chemical analysis of organic light-emitting diodes

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Abstract:

Since their invention in 1987 by Tang and Van Slyke [1], OLEDs have been commercialized for 20 years. This rapid progression to commercialization have been possible by the remarkable research effort to improve OLEDs performances: device lifetime and efficiency. New structures, molecules and the use of dopants allowed this improvement. In the same time, the analysis of degradation in OLEDs by different techniques provided a good tool to understand the weaknesses of OLEDs after aging. The analysis of thin multilayers (100 nm in total) requires the use of instruments with good depth resolution as well as the capacity to detect small chemical changes from aging. Time of flight secondary ion mass spectrometry (TOF-SIMS) and X-ray photoelectron spectroscopy (XPS) have been used to characterize the chemical degradation by providing elemental and molecular information. However, few studies correlate the two techniques.

We developed a protocol for correlative analysis of multilayers by TOF-SIMS and XPS. A bevel crater is formed by varying the fluence of an Argon cluster sputter beam over the surface of the OLED. By analyzing the surface of the same bevel crater, it is possible to correlate the information from the two techniques. In TOF-SIMS, a scan of the surface of the wedge crater provides molecular mapping of molecular ions and characteristics fragments. In XPS, a line scan along the crater allows the identification of the different layers to acquire high-resolution spectra in each layer. This method enables an easy correlation between TOF-SIMS and XPS results and reduce analysis and sputtering damage of buried layers.

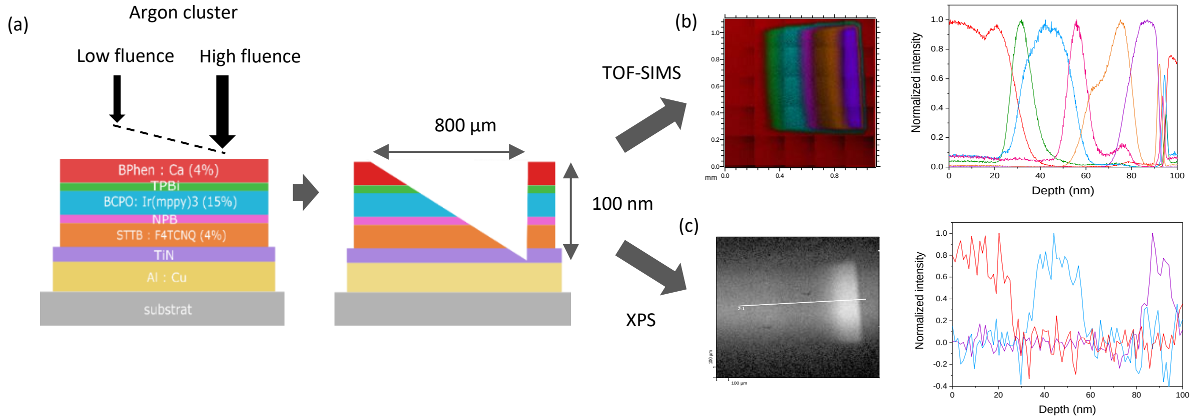

Figure 1. Protocol for correlative analysis of OLED's multilayers [2] (a) formation of crater, (b) TOF-SIMS measurements and (c) XPS measurements

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Poster

Ratiometric Ln^{3+}-based Luminescent Thermometers

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Abstract:

Temperature is a key parameter of many natural and artificial systems. Although several readout methods have been developed through time, nowadays technologies increased the demand to develop new methods with high precision down to the micro and nano-scales. In this respect, luminescent thermometers have been emerged in the studies showing high sensitivity, spatial resolution, fast response, in addition of being non-invasive. Among this family, Ln^{3+}-based luminescent thermometers take a great interest due to the unique photo-physical properties of lanthanides originated from the shielded f orbitals[1].

We will present the first results of our work on the design of ratiometric Ln^{3+}-based luminescent thermometers with performance based on following the variation in the intensity ratio of two Ln^{3+} emitting centers (Eu^{3+} and Tb^{3+}). The transfers of energy in between both emitting species were controlled, thanks to the appropriate design of the ligand regarding the different excited states involved in the process[2]. These thermometers have a simple and easy processibility compared to previously reported systems, prepared by simply mixing complexes of the two Ln^{3+} centers. In addition, these thermometers show a promising performance as temperature sensors in the physiological range (298-323K) making them possible candidates for future intracellular mapping of temperature, a parameter affecting the biological processes.

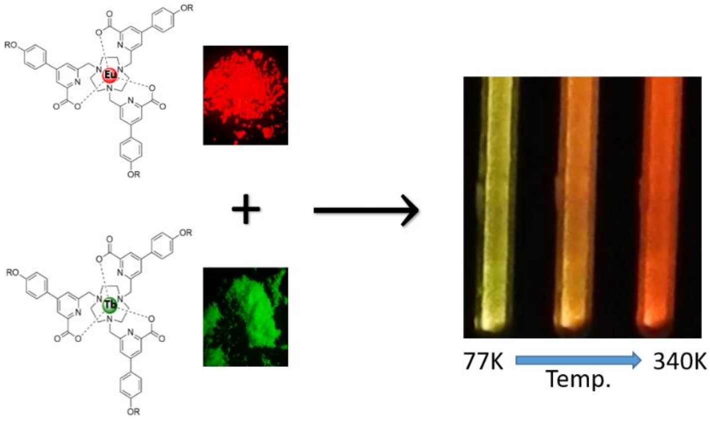

Figure 1: *Color changes (under UV light 365nm) of* Eu^{3+} *and* Tb^{3+} *complexes mixture upon heating.*

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Poster

3,6-Di-*tert*-butyl-carbazolyl-disubstituted trifluoromethyl benzene as multifunctional emitter for colour-tuneable OLEDs

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OLEDs are widely used not only in displays, but also for lighting applications. In the latter case, the desired emission is commonly white one, instead of the primary red, green, and blue emitting OLEDs used in display industry[1,2]. OLEDs are also applied in some other promising fields such as biological sensing, excitation light sources, information storage[3]. Ultra-violet (UV) OLEDs with a emission wavelength (λ_{em}) less than 400 nm are highly demanded in these fields[4]. Only host: guest systems have been used to obtain effective UV-OLEDs so far. The reports on UV-emissive materials are still extremely scarce due to the particular challenge of such compounds to have super wide band gap for exciton confinement within emitting layer to be successfully employed in UV-OLEDs.

Herein, we present theoretical and experimental investigation of new easily obtainable compound 3,6-di-tert-butyl-carbazolyl-disubstituted trifluoromethyl benzene that was used for the fabrication of various types of OLEDs, i.e., exciplex emission based, UV- and white ones.

Acknowledgment. This research has received funding from European Social Fund (project No 09.3.3-LMT-K-712-19-0033) under grant agreement with the Research Council of Lithuania (LMTLT).

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Poster

Correlation between nanoscale thermal and electrical conductivity in PEDOT:OTf thin films

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Conducting polymers are emerging as promising candidates for low cost thermoelectric (TE) devices. Recently, thin films of poly(3,4-ethylenedioxythiophene) (PEDOT) stabilized with trifluoromethanesulfonate (OTf) counter-ions have demonstrated exceptionally high electrical conductivity exceeding 3000 S cm^{-1} [1], which makes it an excellent candidate for potential TE applications. We have used scanning probe microscopy in order to investigate the interplay between electrical and thermal transporting properties of PEDOT:OTf films on nanometric scale. C-AFM allowed us to measure electrical conductivity in out-of-plane direction and revealed significant (about 2 orders) anisotropy due to edge-on orientation of PEDOT chains on the substrate. Null-Point (NP) SThM [2] was used for characterization of local thermal conductivity which demonstrated non-negligible electronic thermal transport in PEDOT:OTf. We modulated electrical conductivity of PEDOT:OTf thin films by employing different co-solvents during deposition as well as reducing agents for post-deposition treatment (de-doping). We measured out-of-plane thermal conductivity values for PEDOT:OTf samples with a wide range of electrical conductivities (0.04-140 S cm^{-1}), for the purpose of estimating the electronic contribution to the thermal transport in this material (Figure). We found a vibrational thermal conductivity of 0.34 ± 0.04 W m^{-1}K^{-1}. From the linear dependence or the electronic contribution of thermal conductivity vs. the electronic conductivity (Widemann-Franz law), we infer a Lorenz number of 1.66×10^{-7} W Ω K^{-2}, larger than the classical Sommerfeld value as also observed in many organic materials [3] for in-plane thermal transport. Applying the recently proposed molecular Widemann-Franz law [4], we deduced a reorganization energy of 0.57 eV, a value higher than expected. We conclude that these approaches need to be refined for the case of highly conductive organic polymers.

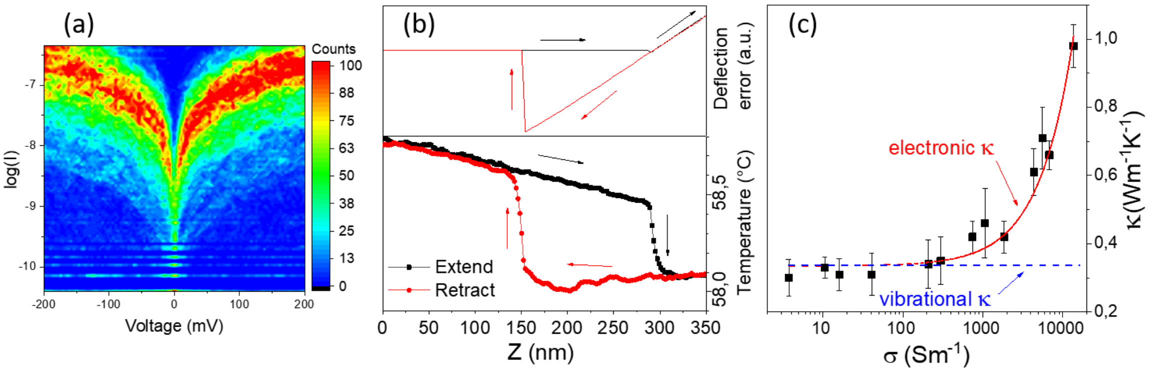

Figure: (a) 2D histogram of 100 C-AFM I-V ramps for pristine PEDOT:OTf; (b) example of NP SThM temperature measurement; (c) plot of out-of-plane thermal conductivity κ as a function of electrical conductivity σ for PEDOT:OTf samples

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POSTER SESSIONS

Wednesday, December 1, 2021

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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
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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
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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
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PO94 - T3 - David Kreher - New LC semiconducting (PBTTT)-based polymer : from synthesis to organic FET properties

Poster

Study in operando of organic semiconductor stretchability

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Abstract:

Stretchability of organic semi-conductors (OSC) is investigated for few years for applications in wearable electronics or electronic skin [1] thanks to their mechanical capacity compared to their inorganic equivalent. This study aims at understanding the link between OSC structural and morphological properties (crystallinity, alkyl chain length, Mw…) and their electrical and mechanical properties. Advanced mechanical, electrical and optical characterizations are carried out in operando on a specific homemade tensile bench to investigate OSC properties under traction. Mainly, a TLM (Transfer Length Measurement) structure with gold electrodes is used to follow contact and OSC resistivity during lengthening. The traction is realized with a micrometric plate, electrical measurements are made with a switching card and a multimeter, and a camera allows to measure at each moment the distance between the electrodes. We choose to study P3HT(poly(3-hexylthiophene)), which is a well documented material. The fact that it can be obtained in amorphous or semi-crystalline form (regiorandom or regioregular) and for various molecular weights [2-4] makes the P3HT a good candidate for our study on the link between polymer structure and mechanical properties. The organic semiconductors used during this study are the 5 poly-thiophenes P3xT, with x : hexyl, octyl, decyl, dodecyl, butyl.

As the OSC used in this study are soluble in chlorinated solvent, which damage the stretchable silicone based substrates (PDMS: Polydimethylsiloxane) used, a transfer technic using a sacrificial layer has been developed to transfer OSC on the stretchable substrate. Besides protecting the substrates from solvent, transfer technic also allows to drop off OSC on a pre-constrain substrate to gain few level of stretchability. [5]

Electrical, mechanical and morphological characterizations will make it possible to make the link between the structure of the OSC films and their mechanical and electrical properties.

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Poster

Gas sensors based on nano molecular electronic devices

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Abstract:

When miniaturizing gas sensors, chemiresistors are an excellent choice since those sensors can have a nanometer to micron size, and the transducer unit is addressed by an electrical connection which enables easy integration with other electrical components. Classical chemiresistors consist of metals, metaloxides or polymers. Whereas metals are mainly used for selective detection of very few gases such as for example H_2, metaloxides and polymers are sensitive to a large variety of gases though the disadvantage of metaloxide thin film based sensors is their low relatively low selectivity to different gases [1]. Polymer based sensors can be more selective and equally operate at room temperature. Though, since gases diffuse into the polymer and bind to the molecular chains, the sensors have a short lifetime [2], the response of a polymer based gas sensor is a complex function of [D. W. Hatchett, M. Josowicz, Chem. Rev. 2008 , 108 , 746 .], the modification of both, the structure of polymer sensors as well as a modification of the electronic structure of the gas sensor molecules upon interaction with the sensing gas. A more straightforward situation can be created when conductive gases interact directly with free-standing conjugate molecules being contacted to metallic electrodes such as in [1-5]. In this case, the NO_2 gas sensor response could be directly explained by the change of the density of states and the corresponding transmission function followed by adhesion of the gas to the molecule.

Here, we use a simplified method to synthesize the AuNPs and demonstrate that the gas sensor response to NO_2 gas also is present on those modified nanoMoED devices using 1,8 biphenyl-dithiol (BPDT) molecules. We carry out NO_2 gas sensor experiments with several sensor molecules to test alternative molecules that equally contain phenyl rings. The selectivity of the BPDT molecule towards different gases is addressed by using this device platform for NH_3 sensing.

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Poster

Trap characterization in disordered organic semiconductors by Q-DLTS

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Abstract:

The presence of traps in organic semiconductor based electronic devices affects considerably their performances and their stability. The Shockley-Read-Hall (SRH) model is generally used to extract the trap parameters from the experimental results. A new model is proposed to describe defect states in disordered organic semiconductors. We adapt the SRH formalism to disordered organic semiconductors by considering a hopping transport process and Gaussian distributions for both mobile and trapped carriers. We used the approach of Kuik *et al.* [1] to calculate the capture frequency. The capture, c_n, and the emission frequency, e_n, of a discrete trap contribution becomes: $-$ and $-$ —— . The relaxation of the trapped charges is given by $Q_t(t) = Q_{t0}\exp(-e_n t)$. In this study, we have used the advanced mobility model of Oelerich *et al.* [2] [3].

The model is used to extract multiple trap parameters from charge based Deep Level Transient Spectroscopy (Q-DLTS) spectrum. The model fits the Q-DLTS spectra measured on a perovskite based N-I-P solar cell structure [4]. For each trap distribution, trap parameters were extracted. Good agreement with experimental data is obtained (Fig. a). The reliability of the extracted values will be discussed with respect to various unknown parameters of the sample. We will show that the LUMO width, i.e., the rate of disorder of the organic material, is the most sensitive parameter. The width of the LUMO influences the positions of the trap energy levels but not their own distribution widths. The trap distributions are found closer to the transport band when the degree of disorder is high with relatively large DOS (Fig. b). Analysis of the reliability of the extracted trap parameters emphasized the need of a better knowledge of the LUMO characteristics. The present model is based on the most advanced transport model in disordered semiconductors and represents a significant step towards accurate trap characterization. This work is expected to help understanding some experimental results of disordered semiconductor.

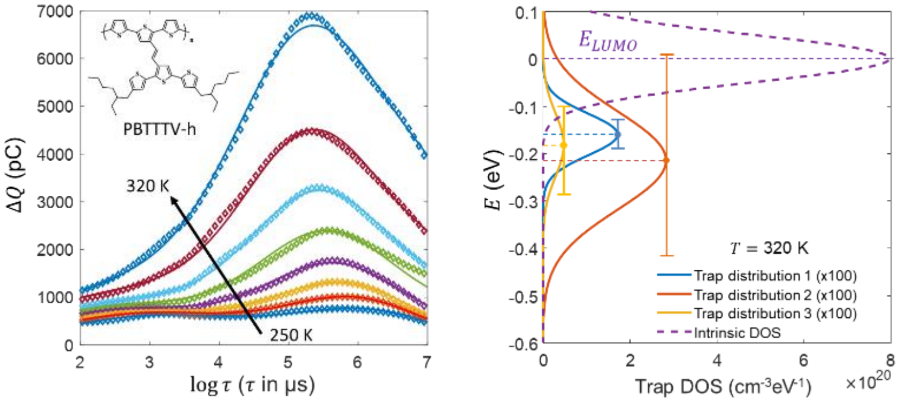

Fig. a) Experimental (symbols) from [4] *and simulated Q-DLTS response (plain lines) and three Gaussian trap contributions. b) Representation of the DOS of the three trap contributions at 320 K.*

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Poster

Synthesis and studies of differently substituted triazatruxenes for organic optoelectronics

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Abstract:

10,15-dihydro-5H-diindolo[3,2-a:3',2'-c]carbazole also known as triazatruxene is electron rich compound. Materials on its basis are explored for the devices of organic optoelectronics such as solar cells and organic light emitting diodes. N,N,N-trialkyl substituted triazatruxenes containing aromatic substituents at 3,8,13 positions were widely explored and reported. In contrast, N,N,N-triaryl substituted triazatruxenes were described only in a few papers. Derivatives of triazatruxene described earlier exhibited high hole drift mobilities and good thermal and morphological characteristics which made the promising materials for organic optoelectronics[1-5].

The derivatives of triazatruxene, which will reported in this presentation, were synthesized from triazatruxene and the corresponding halogenated compounds by Buchwald-Hartwig coupling with moderate or high yield. All the synthesized materials were amorphous. They exhibited very high thermal stability with the temperatures of onsets of thermal degradations above 400°C and high glass transition temperatures. The dibenzotiophenyl substituted triazatruxene exhibited glass transition temperature of 227 °C. The highest holes mobility of $1.6\cdot10^{-3}$ cm^2/Vs at 766 $V^{1/2}/cm^{1/2}$ showed N-phenylcarbazolyl substituted triazatruxene. The triplet state energies of the derivatives were in the range of 2.64-3.00 eV.

Acknowledgment :

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Poster

The defects in the organic spin chain compounds (o-DMTTF)$_2$X (X= Cl, Br and I) : a system behaving like a molecular magnet

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The organic compounds (o-DMTTF)$_2$X crystallise in a tetragonal structure, two molecules of DMTTF and a counter-anion X share an electronic lack of spin ½. The electronic spins are strongly coupled by an Heisenberg exchange along the c axis. This system is a model to the study of antiferromagnetic Heisenberg spin chains. Below the temperature T_{sp} the spin Peierls transition occurs: the spin chains become dimerized and an energy gap between the ground state and a continuum of energy is created. As a consequence of the dimerization the ground state should be non magnetic. A non magnetic defect like a break in the translationnal symmetry induces a magnetic ground state made of tens of spins [2,3]. By means of Electron Spin Resonance spectroscopy we have measured these intrinsic defects and their quantum coherence, a prerequisite for quantum processing [3]. The term molecular magnet usually refers to a cluster with several magnetic ions strongly coupled by exchange interactions like V_{15}, Mn_{12} or Fe_8 [4,5,6]. In this poster we show that the defects in dimerized spin chains and molecular magnets have many similarities.

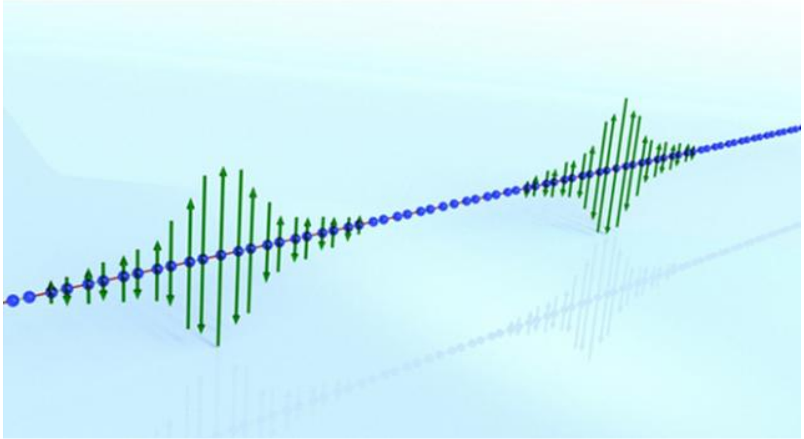

Figure 1 – Artistic view of strongly correlated defects in dimerized spin chains

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Poster

Electrochemical sensing of naphthalene based on a renewable graphene oxide paste electrode

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Abstract:

A graphene oxide paste electrode (GO-CPE) based on 5,10,15,20-tetrakis(4-methoxyphenyl)-21H,23H-porphine nickel (II) and N-(1-Naphthyl)ethylenediamine dihydrochloride was constructed and used for the electrochemical detection of naphthalene (NAP). Taking into consideration the unique π-π stackings between N-NEDDH and naphthalene a selective and sensitive electrode was constructed. The electrochemical behaviour of the modified N-NEDDH/NiTPP/GO/CPE was studied by cyclic voltammetry (CV), electrochemical impedance spectroscopy (EIS) and differential pulse voltammetry (DPV). Under the optimal conditions, the modified sensor presented a wide linear concentration range from 1×10^{-8} to 1×10^{-5} mol L^{-1} in the detection of naphthalene, with a 3×10^{-9} mol L^{-1} detection limit. Other PAHs, like phenanthrene, anthracene, fluorene and pyrene showed little interference on the detection. It also demonstrated a good applicability on naphthalene determination from four types of water samples, with good recovery rates.

Poster

Electrical characterizations of individual supramolecular crystals at the local scale

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Abstract:

The development and improvement of organic electronic devices requires analytical tools allowing for a deep understanding of the physical properties of the materials they are made of. Bulk characterization techniques only offer ensemble-averaging information that does not take into account the heterogeneity of the samples (defects, polymorphism, grain boundaries in polycrystalline materials, anisotropy…). The fabrication of devices on every region of interest of a sample is an extremely tedious and time consuming task. There is therefore a need for developing tools to probe locally the materials. In order to study the structure-property relationship, it is also important for these tools to be adaptable to other characterization techniques allowing correlative measurements.

In this contribution, the use for electrical measurements of a nanoprobing station consisting of four IMINA® nanorobots will be presented. The nanorobots can be equipped with tungsten tips that can thus be manipulated to contact any location of a sample at will, with a precision down to 10 nm. A proof-of-concept will be given by the study of supramolecular crystals of a thienopyrroledione (TPD) - triazatruxene (TAT) derivative (figure 1a), a molecule used in photovoltaics [1]. The probes are used in the environment of a scanning electron microscope (SEM) to contact on demand single crystals in various configurations (field-effect transistors, 4-probe measurements) to measure the electrical properties (such as mobility) of individual supramolecular objects. The possibilities of development for other types of materials and in other environments will be discussed.

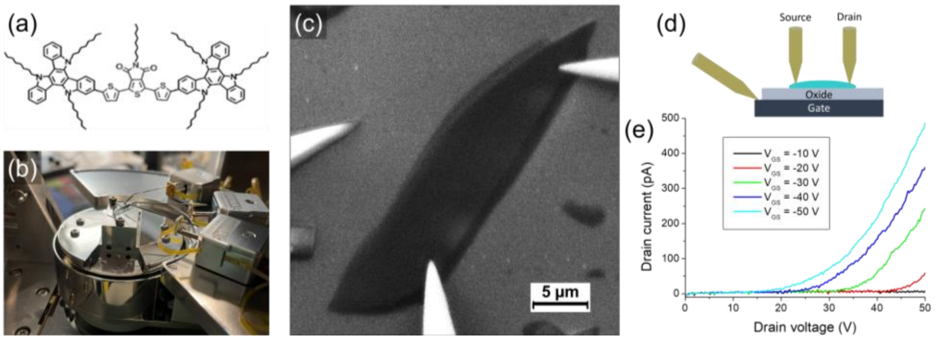

Figure: (a) structure of the TPDC8-TATC8 molecule; (b) photograph of the nanoprobing stage equipped with three robots and a sample placed on a cryo/heating module (range: -190°C to +300°C); (c) SEM image of a TPDC8-TATC8 supramolecular crystal contacted by two probes (source and drain); (d) diagram of experimental setup using three probes in a back-gate FET configuration; (e) output characteristic of a TPDC8-TATC8 crystal.

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Poster

Organic Phototransistor based on oriented thin film of Poly (3-hexylthiophene)

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Abstract:

Organic semiconductor based field effect transistor have a broad range of application in various type of sensor including light sensor, pressure sensor, gas sensor and chemical, biological and medical sensors. Among the photo detectors, OFETs based phototransistor have the advantages over the others in limiting the dark current and improved signal to noise ratio and high sensitivity.

We have studied, poly (3-hexyl thiophene) based OFETs under the light illumination, as well as performance of these device as a phototransistor. For high performance and low cost, a novel proposed ribbon-shaped FTM have be used for thin film deposition of the polymer. The prepared film is oriented and investigated by calculating the dichroic ratio (DR). The highly oriented film shows the dichroic ratio DR ~ 2, and used as an active semiconducting material by fabricating the OFETs in bottom gate bottom contact (BGBC) configuration. OFETs performance was calculated by drain current at saturation and showing the average field effect mobility (μ) 6×10^{-3} cm^2/vs and Ion/Ioff ratio = 2.4×10^3. The device measured in air at ambient condition. Interestingly, a mobility of parallel oriented thin films prepared by ribbon-shaped FTM was about more than one order of magnitude higher compared to the OFETs fabricated using conventional FTM (7.22 x 10^{-4} cm^2/Vs). Further, OFETs observed under illumination of light (λ=550 nm, Pin= 0 to 1.10mW/cm^2) and showing the amplified drain current I_{DS} and change in the threshold voltage shown in figure 1. We will also discuss the of photosensitivity and responsivity of the oriented film during the presentation.

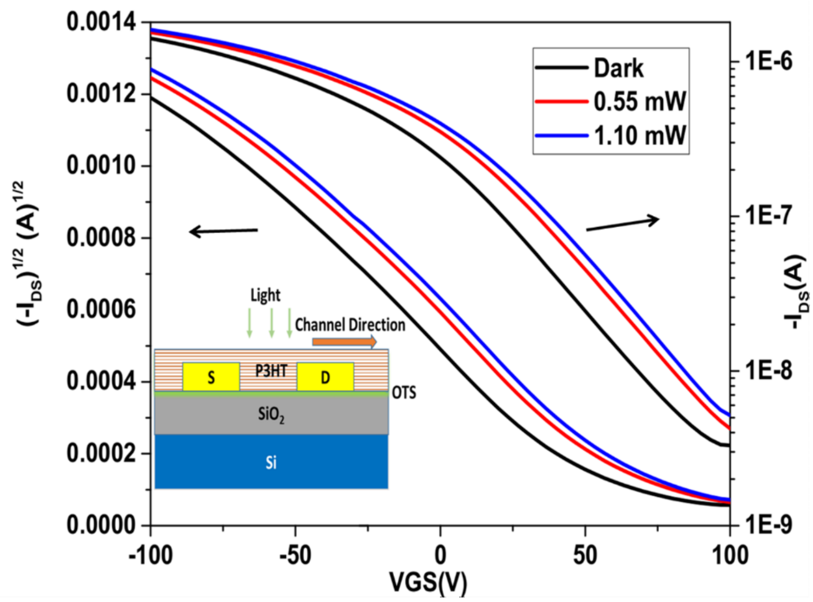

Figure-1 Transfer characteristics of organic phototransistor measured under light illumination from the light intensity 0 to 1.10 mW/Cm^2

Poster

TADF properties of derivatives of phenothiazine or phenoxazine-substituted benzanthrones emitting in deep-red/near-infrared region

Uliana Tsiko, Oleksandr Bezvikonnyi, Dmytro Volyniuk, Viktorija Andruleviciene, Asta Dabuliene, Juozas Vidas Grazulevicius

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Abstract:

The development of new materials demonstrating red and near-infrared (NIR) emission has attracted the attention of the researchers over the last two decades due to the number of possible applications in bioimaging, photodynamic therapy, sensors, information-secured displays, night vision devices and optical telecommunications.[1,2]. Such a broad area of the possible applications of NIR emission in organic electronics stimulates the development of new devices exhibiting NIR electroluminescence (EL) [3]. In addition to the above mentioned conventional applications of thermally activated delayed fluorescence (TADF) emitters, they have also significant potential to be used as active indicators (luminescent probes) in optical oxygen sensors.

Aiming to develop new deep-red/near-infrared emitters, benzanthrone as a new acceptor moiety with a rigid molecular structure was used. For the design of target compounds phenothiazine and phenoxazine moieties with strong electron-donating ability were also used. Such combination allowed new materials demonstrating TADF in the long wavelength region to be obtained. The maximum intensity of fluorescence of the solid samples of the synthesized compounds was observed at 700 nm. EL was peaked at similar wavelength when the compounds were used as emitters for the fabrication of non-doped organic light-emitting diodes. The film of molecular dispersion of phenoxazine containing compound in inert polymer ZEONEX® was used for estimation of oxygen sensing ability. The ratio of intensity of TADF taken in vacuum and of prompt fluorescence taken under oxygen purge was found to be ca. 15.2. The oxygen sensitivity of the film estimated by Stern-Volmer constant was found to be of 1.6×10-4 ppm-1.

Acknowledgement

This project has received funding from European Regional Development Fund (project No 01.2.2-LMT-K-718-01-0015) under grant agreement with the Research Council of Lithuania (LMTLT)

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Poster

Photophysical and electroluminescent properties of non-planar pyridines ornamented with multiple donor moieties

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Viktorija Andrulevičienė,[a] Uliana Tsiko,[a] Egle Jatautiene,[a] Sergey Belyakov,[b]
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Abstract:

Organic light-emitting diodes (OLEDs) have big potential to be applied in modern display and lighting technologies [1]. The most efficient OLEDs are based on emitters having ability to harvest singlet and triplet excitons including materials exhibiting thermally activated delayed fluorescence (TADF).

Many efficient TADF emitters were developed exploiting multiple-donor-acceptor molecular structures with one-type of donors and acceptors [2]. To study effect of different types of donors in the structures of organic emitters on their TADF properties, two multiple-donor-substituted dicyanopyridines with three donors of one-type (3,6-di-*tert*-butyl-carbazolyl) or two-types (3,6-di-*tert*-butyl-carbazolyl and phenothiazinyl) in their molecular structures were developed [3].

The compound with one-type of donor exhibited only conventional TADF. Meanwhile, the compound with two-type of donors showed the conventional and dual TADF. The dual TADF resulted from recombination of two different intramolecular charge transfer states. OLEDs with phenothiazinyl and 3,6-di-tert-butyl-carbazolyl containing emitter exhibiting dual TADF showed low device life-times and low maximum external efficiency of 3.1 % for the non-doped device and of 5 % for the doped device. Low efficiency of dual TADF based OLEDs is attributed to the additional energy transfer with quantum yields lower than 100%. In addition, the device stability and efficiency were partly affected by ultra-long emission life time (up to milliseconds) which can enhance probability of exciton-exciton and exciton-polaron annihilations under electrical excitation. In contrast, non-doped and doped OLEDs based on the 3,6-di-tert-butyl-carbazolyl multiple substituted dicyanopyridine showed relatively high device life-times and high maximum external efficiency of 8.1 and of 25 %, respectively.

Acknowledgements

This project has received funding from European Regional Development Fund (project No 01.2.2-LMT-K-718-01-0015) under grant agreement with the Research Council of Lithuania (LMTLT).

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Poster

Designing ferromagnetic metal/molecule interfaces to preserve molecular functionality

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Abstract:

The study of the spin properties of ferromagnetic metal-organic interfaces has recently received considerable attention because of the prospect of developing new hybrid and multi-functional molecular devices. As an important development, recent research has shown that the interface between a ferromagnetic (FM) metal and molecules is highly spin-polarized at room temperature. This feature of the so-called 'spinterface' [1] is evident in spin-polarized photoemission spectroscopy [2,3] and magnetotransport experiments [4,5]. At stake is a higher spintronic performance that benefits not only information encoding [6], but also energy harvesting [4,5] strategies (www.spinengine.tech).

After reviewing the state-of-the art regarding the spinterface, including recent experiments into its origin [3], we will present a strategy [7,8] to preserve the fragile electronic property of functional molecules, such as spin crossover (SCO) complexes [9], upon forming the spinterface. Here, the FM metal and molecule are separated by an ultrathin noble metal (NM) spacer layer (Cu, Au). Thanks to the physics of giant magnetoresistance [7] and spin-polarized charge transfer [8], the magnetism of the molecule is controlled by the FM layer across the NM layer. This strategy can ultimately enable a wide range of molecules to act as single molecule magnets, at much higher temperatures than reported [10]. Finally, we have performed device in operando experiments using synchrotron radiation to factually demonstrate [11] that the SCO property is involved in electrical transport. Our experiments thus shed light into the actual transport path across the SCO thin film.

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Poster

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.

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Abstract:

Doping polymer semiconductors is a central topic in plastic electronics and especially in the design of novel thermoelectric materials. In this contribution, we demonstrate that doping of oriented semi-crystalline P3HT thin films with the dopant tris(4-bromophenyl)ammoniumyl hexachloroantimonate), also known as magic blue, helps reach charge conductivities of 3000 S/cm and thermoelectric power factors of the order of 180 μW/mK^2 along the polymer chain direction. A combination of transmission electron microscopy, polarized optical absorption spectroscopy and TE property measurements helps clarify the conditions necessary to achieve such high charge conductivities.[1-3] The mechanism of doping is intimately related to the semi-crystalline structure of the polymer and whether crystalline, amorphous or both phases are doped.[2] In the case of MB, mainly amorphous P3HT domains are doped while the structure of crystalline P3HT domains is almost unaltered by doping. A comparison with other dopants such as $FeCl_3$, F_4TCNQ, F_6TCNNQ and Mo(tdf-COF_3)$_3$ indicates that the highest charge conductivities are obtained when the only amorphous phase of P3HT is preferentially doped. Charge transport improves in the sequence: i) doping of the only crystalline phase (F_6TCNNQ and F_4TCNQ), ii) doping of both crystalline and amorphous phases ($FeCl_3$, Mo(tdf-COF_3)$_3$) and iii) doping of the only amorphous phase (Magic blue).

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November 29 - December 2, 2021
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Poster

Para-azaquinodimethane: New building block for optoelectronic applications

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Abstract

The quinoidal structure is an interesting entity with unique optical, magnetic and electronic properties[1]. In contrast to their aromatic counterparts, quinoids show significant bond length alternations that break the aromaticity, reduce the highest occupied molecular orbital (HOMO)–lowest unoccupied molecular orbital (LUMO) gaps that potentially enable injections of both electrons and holes, different chemical reactivities and low-symmetry spectroscopic features that guarantee new functionalities[2]. Quinoids are characterized by rigid and coplanar structures and excellent delocalization of π electrons which leads to efficient charge transport[3]. Among different quinoidal building blocks such as benzodipyrrolidone (BDP)[4], naphthodipyrrolidone (NDP)[5] , benzo[1,2- b:4,5-b']-dithiophene-2,6-dione (BDTD)[6] and para-azaquinodimethanes (*p*-AQM)[1,2]; *p*-AQMs show remarkable advantages. The combination of facile synthetic accessibility, high chemical stability, small optical band gaps, tunable optoelectronic properties, and good electronic performance[1] makes *p*-AQM promising building blocks in low band gap polymers, organic electronics and thermoelectric devices[7] . Herein, we study a new family of *p*-AQM molecules starting from cyclic aryl ketone precursors, where the choice of ring system affects structural rigidity[8]. The *p*-AQM unit is synthesized by knovenagel condensation followed by alkylation as shown in figure 1. The introduction of electronegative nitrogen atoms in the central core play multiple roles of electronic and steric effects[2] while the alkoxy substituents have an influence on the solubility and stability of the molecules [1].Furthermore, the regioselectivity of symmetrical ketones and the possibility of different substitution patterns of the aryl moiety offer a synthetic variety of target molecules. In brief, our work is an ongoing research on the future of ketone-based *p*-AQM structures for various optoelectronic applications.

Keywords: quinoidal structure, p-AQM, knovenagel condensation, cyclic ketones.

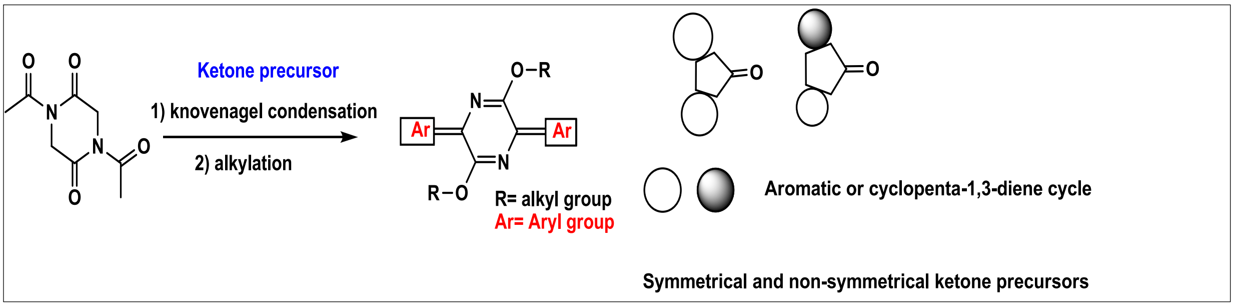

Figure 1: General synthetic method to p-AQM and cyclic ketone precursors

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Poster

Effect of Cr content on structural, microstructural, magnetic and hyperfine properties of nanostructured $(Fe_{0.7}Co_{0.3})_{100-x}Cr_x$ alloys

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Abstract:

In this work, we have studied the effect of Cr content on the structural, microstructural, magnetic and hyperfine properties of the nanocrystalline ternary FeCoCr system. The $(Fe_{0.7}Co_{0.3})_{100-x}Cr_x$ (x = 0, 5, 10, 15 and 20 at.%) powders were elaborated by high energy ball alloying for a milling time of 72 h. X-ray diffraction (XRD), scanning electron microscopy (SEM), ^{57}Fe Mössbauer spectroscopy at 300 K

and vibrating sample magnetometry (VSM) have been used to investigate the physical properties of elaborated $(Fe_{0.7}Co_{0.3})_{100-x}Cr_x$ alloys. X-ray diffraction patterns show the formation of a disordered bcc Fe (Co, Cr) solid solution. The lattice parameter, a (Å), the lattice microstrain ε (%) and the coercive field H_C increase up to a critical Cr content (x_{crit}= 10 at.%), beyond the critical content, these parameters decrease progressively with increasing Cr content. The average grain size, D (nm), decreases to 65 % of its initial value (x= 0 at.%) after an addition of Cr to the elaborated compositions. The SEM photographs show the variation in the in particle size, shape and morphology, when the Cr content increases. Quantitative EDX analysis confirms the absence of the contaminants and the starting stoichiometry conservation. Therefore, the saturation magnetization value decreases almost linearly by adding Cr to the composition. Mössbauer results will be discussed as a function of Cr content.

Poster

Screening of the synthesis route on the structural, magnetic and magnetocaloric properties of $La_{0.6}Ca_{0.2}Ba_{0.2}MnO_3$ manganite: A comparison between solid-solid state process and a combination polyol process and Spark Plasma Sintering

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abstract

$La_{0.6}Ca_{0.2}Ba_{0.2}MnO_3$ ceramics are prepared by an original route, combining soft chemistry and Spark Plasma Sintering, within a few minutes at 700 °C and by the solid-state reaction at high temperatureswith an annealing temperature of 1200 °C. We have studied the leverage of the powder synthesismethod on the structural, morphological, magnetic and magnetocaloric properties of the samples. X-ray diffraction analysis using Rietveld refinement revealed that our materials crystallize in the rhombohedral system with R3-c space group for the sample prepared by the Polyol-Spark Plasma Sintering method and in the orthorhombic structure with Pbnm space group for the sample synthesized by the solid-state reaction. Magnetization measurements versus temperature under

magnetic applied field of 0.05 T show a paramagnetic-ferromagnetic phase transition for both samples. The Arrott plots reveal that ours materials undergo a second-order phase transition. The maximum values of the magnetic entropy change ($-\Delta S^{max}{}_{M}$) under the magnetic field change of 5 T are 2.4 and 4.7 J/kg K for $La_{0.6}Ca_{0.2}Ba_{0.2}MnO_3$ synthesized by using solid-state reaction and Polyol-Spark Plasma Sintering methods respectively. The highest value of the relative cooling power RCP is

found to be 244 J/kg for the Polyol-Spark Plasma Sintering sample under 5 T. These re

interesting enough and suggest that the Polyol-Spark Plasma Sintering synthesis method is a feasible

route to prepare high quality perovskite material for magnetic cooling application.

Keywords: Manganites, Preparation methods, Magnetization, Magnetocaloric effect


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Poster

Non-covalent assemblies of carbon nanotubes and cobalt corroles applied to oxygen reduction reactions (ORR)

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Abstract:

As the need for more effective and greener energies grow to resolve the environmental problematic of this century, a solution has come with the development of fuel cells. Based on the exchange of protons through a membrane to reduce dioxygen, it uses gas and produces water as its only waste material. Considering the cost of the platinum electrode used in these systems, the search for non-noble metal effective and selective catalysts is still an ongoing challenge. Cobalt based macromolecules such as corroles have proved to be effective for Oxygen Reduction Reaction (ORR)[1,2,3], and especially when combined with carbon nanotubes.[4] More recently, polymerization of cobalt porphyrins around nanotubes gave higher ORR efficiencies than the simple adsorbed system.[5] Combining these two results, this presentation will focus on the preparation and electro-catalytic activities of the first examples of hybrid systems where cobalt corroles are polymerized around multi-walled carbon nanotubes thanks to multiple click reactions.

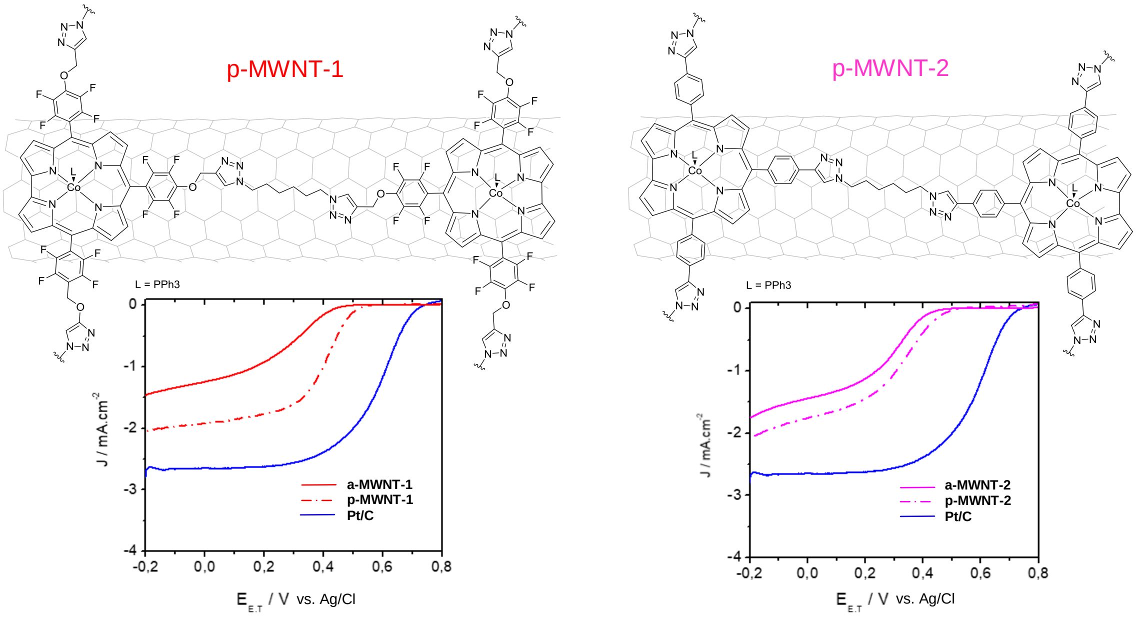

Figure 1: Cobalt corroles polymerized on carbon nanotubes systems and their rotating ring-disk electrode curves (rotation at 800 rpm at pH 0)

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Poster

Hybridization and thermoelectric effects in WSe_2 based transistors

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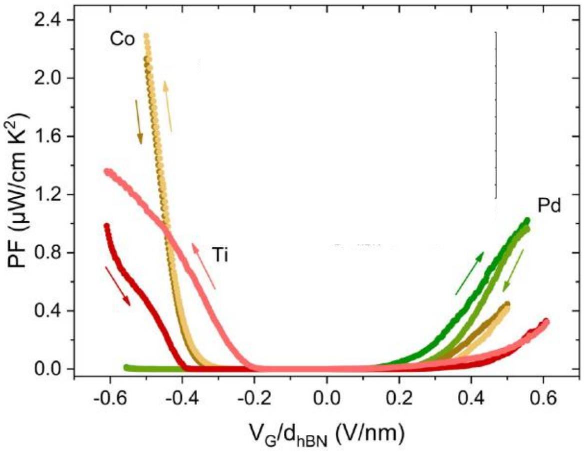
Abstract:

In transistors based on transition metal dichalcogenides (TMD) such as MoS_2 or WSe_2, hybridization between the atoms of the metal contacts and the atoms of the two-dimensional semiconductor plays a key role in the electronic transport properties. It can induce localized states at the edges of the valence and conduction bands and strongly influence the band structure [1]. Here we report on the measurements of the thermoelectric properties of hBN-supported few layers WSe_2 transistors fabricated with different metal contacts (Ag, Pd, Co, Ti) [2]. We obtain values of the Seebeck coefficient S up to 180 mV/K and power factors $S^2\sigma$, σ being the electrical conductivity, as high as 3.5 mW/cm K^2 in a agreement with previous results [3]. Our results show that a strong hybridization at the metal/semiconductor interface allows higher power factors and open new routes for improving the thermoelectric response of TMD-based devices.



Power factors for three different metal contacts as a function of the gate voltage V_G normalized to the thickness of the hBN layer d_{hBN}.

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Poster

Probing strain in monolayer MoS_2 by scanning tunneling microscopy induced excitonic luminescence

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Abstract:

Strain engineering has been widely explored to tune the electronic and optical properties of low-dimensional semiconducting materials, such as nanowires [1] and transition metal dichalcogenide monolayers [2]. Strain modulates the band structure, which is conveniently probed by analyzing photoluminescence spectra [3]. In conventional far-field light microscopy setups, however, lateral resolution is limited by diffraction, and strain can only be poorly localized.

In our work, we use the tip of a room-temperature scanning tunneling microscope (STM) as an electron source to excite the sample locally, and detect the light emitted from the tunneling junction. We report on local strain-modulated excitonic luminescence in monolayer MoS_2, with a spatial resolution better than 10 nm. To this end, monolayer MoS_2 flakes were synthesized by chemical vapor deposition and transferred onto an evaporated gold substrate. Van der Waals interactions make the highly flexible monolayer MoS_2 conform to the corrugated surface of the gold substrate, generating local strains (Figure 1a). STM-induced luminescence spectra show significant shifts for both *A* and *B* excitonic emission peaks in regions of high local curvature. We attribute these shifts to the strain, which modulates the electronic band gap and the valence band splitting of monolayer MoS_2 (Figure 1b), and quantify the modulation rates of *A* and *B* exciton energies as -75±12 meV/% and -57±11 meV/%, respectively.

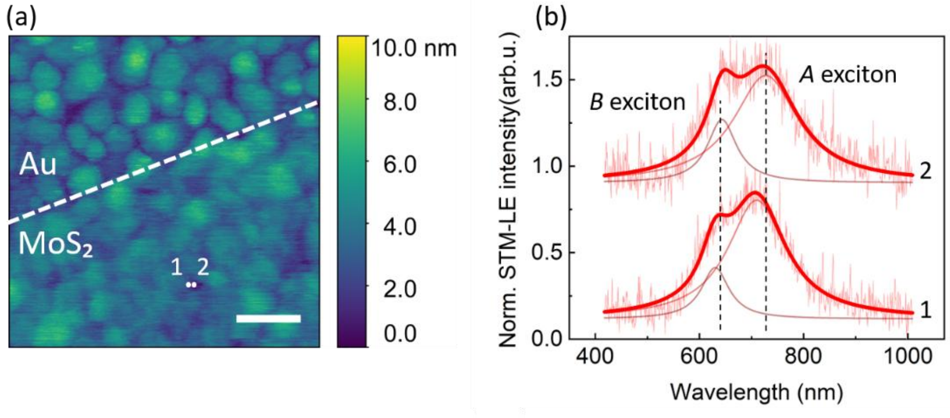

Fig. 1 (a) STM topography of MoS_2 monolayer on Au substrate. Scale bar: 100 nm. (b) STM induced light emission (STM-LE) spectra acquired at the locations marked in (a), with 10 nm separation.

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Poster

Low-temperature transport properties of MoS_2 nanotubes

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Luka Pirker,[b] Maja Remškar,[b] and Andreas K. Hüttel[a]

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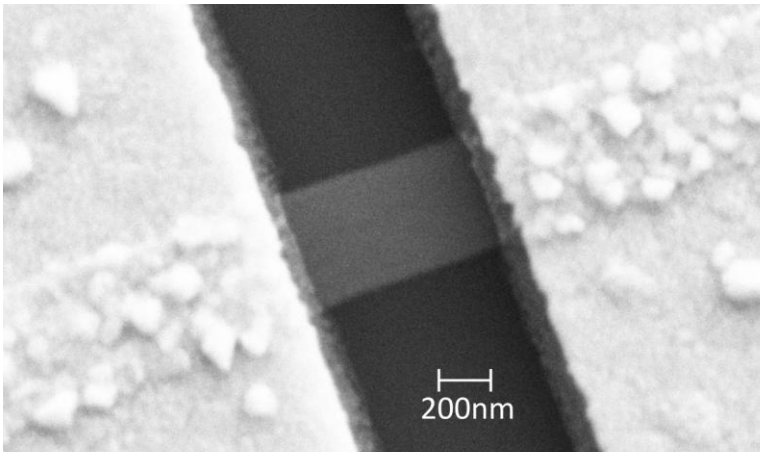
Abstract:

Synthesis procedures for MoS_2 nanotubes and similar materials are well known [1, 2], and many works on the optical response of these nanotubes exist. Even so, their quantum transport properties remain largely unexplored to date. First low-temperature transport spectroscopy results show clear Coulomb blockage at 300mK [3], however, the contact properties are still a limiting factor. While the Fermi level pinning near the conduction band requires low-work function metals such as scandium or titanium for a negligible Schottky barrier, these metals are also reactive and destroy the MoS_2 lattice on contact.

Recently, unprecedented low contact resistance has been demonstrated for the bismuth-planar MoS_2 material combination [4]. Here we present transport measurements on MoS_2 nanotubes with bismuth contacts. Synthesis via a chemical transport reaction yields nanotubes with diameters down to 7nm, lengths up to several millimeters, and an extremely low number of defects. The nanotubes are transferred to a Si/SiO_2 substrate, located with an optical microscope, and contact electrodes are deposited using electron beam lithography. At millikelvin temperatures, the resulting devices display Coulomb blockade, with a rich set of spectroscopic features. In comparison with earlier scandium-based devices [3], disorder is clearly reduced.



Collapsed MoS_2 microtube forming an edge-free nanoribbon

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Poster

Silver nanowires Electrodes and Plasmon resonance influences on Organic Solar Cell Active Layers

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Abstract:

The transparent electrode commonly used in organic solar cells is based on Indium-Tin Oxide (ITO). It contains indium, which is an expensive, rare, difficult to extract and endangered element; hence the need to find an alternative to this electrode. Silver nanowire electrodes have emerged as one of the most attractive alternatives due to their excellent electrical and optical properties [1]. In this work we show that embedding silver nanowires (AgNWs) between two layers of ZnO nanoparticles (ZnoNPs) leads to superior optoelectronic performance compared to a transparent electrode made of ITO. We also highlighted the effect of plasmon resonance related to silver nanowires. An increase in the absorption of an organic solar cell active layer (PCE12:ITIC) is observed. This enhancement is due to the electric field resulting from the plasmonic phenomenon, since the absorption is proportional to the square of the electric field magnitude [2].

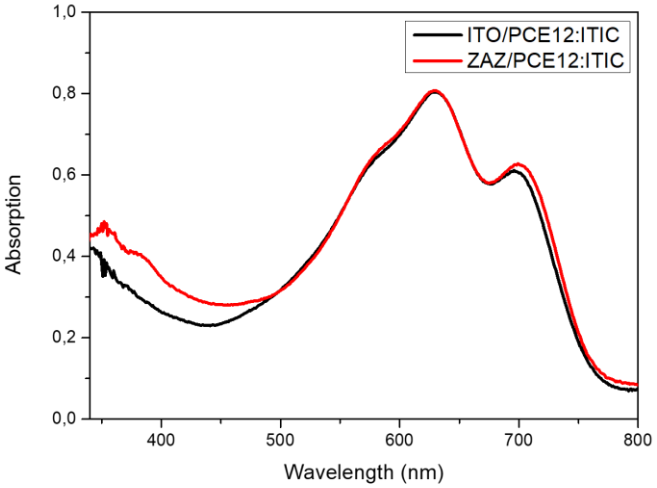

Figure : Absorption of organic solar cell's active layer (PCE12:ITIC) on ITO and ZAZ (ZnO Nanoparticles/AgNWs/ZnO Nanoparticles) electrode.

References:

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Poster

Electron Responsive Viologen-based Supramolecular Gels

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Abstract:

In a nutshell, a gel is a material in which a large amount of solvent is trapped in a molecular network. In supramolecular gels, self-assembly of the network is achieved by non-covalent interactions (π- π stacking, H-bonding, ion pairing, solvophobic forces…) between low molecular weight gelators (LMWGs). Unlike polymeric gelators LMWGs have a well-defined chemical structure, offering the possibility to tune the material properties at the molecular level [1]. Stimuli responsive self-assembled molecular materials are capable of changing their organization in response to various stimuli (pH, T, P, magnetic field, light…). Such responsiveness has been proved useful in numerous fields such as catalysis, smart materials, pollutant removal, drug delivery system, development of sensors and memory devices [2]. However little examples of electro-responsive supramolecular materials are to be found in the literature [3]. The potential of such materials has recently been demonstrated through the development of a gel-based memristor exploiting conductivity changes associated to a sol/gel transition triggered by heating or DC bias [4]. Viologens carry much interest for the development of new functional materials and have already shown promising results for applications in molecular electronics [5]. We have recently reported a supramolecular metallogel able to undergo a gel-sol transition triggered by photo-reduction of its viologen moiety [6][7]. In the wake of this promising result a previously described viologen based gelator [8] has been synthesized and its gelation conditions have been investigated (Figure 1). Rheological and conductivity measurements have shown that gels of tunable strength and conductivity could be obtained. First photoreduction trials have shown that the viologen based gelator could be photoreduced in its gel state, giving a blue coloration to the material.

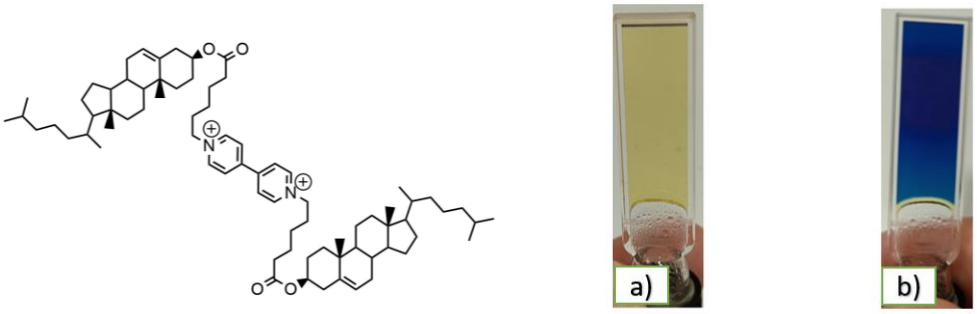

Figure 1 Left: Molecular structure of the investigated viologen. Right: Viologen based organogel: a) Before irradiation, b) After 10 minutes irradiation at 455nm

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Poster

Self-assembly of naphthalene diimide (NDI) within polysilsesquioxane gel

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Gel is a solid-like material composed of a huge amount of solvent entrapped into a 3D network, known as a supramolecular gel when the 3D network is formed by physical interactions between the molecular units or polymer gel when the solvent is immobilized by covalent cross-linked structures [1,2]. In both cases, the organization of building elements within the network is a key element that determines the mechanical and electrical properties of the gel. [2] There is thus a great interest in being able to control or tune the organization of those building elements in order to improve the applicability of polymer gels in areas such as tissue engineering, optoelectronics, catalysis, drug deliveries and so forth [1,2].

Our own work focuses on hybrid gel materials obtained by polycondensation of silsesquioxane R-$[SiO_{1.5}]_n$ ($n \geq 1$). Depending on the nature of the organic group R, physical interactions and steric effects between organic units act as driving forces in the structural organization of the network. Simultaneously, the formation of intermediate silanols can also influence the orientation of the precursors through the formation of intermolecular hydrogen bonds [3,4]. After gelation, the aging period begins, in which phenomena such as densification of Si-O-Si structures, solvent evaporation, reorganization of the 3D network occurs [3]. The objective of our work was to characterize the reorganizations processes occurring within naphthalene diimides (NDI)-containing polysilsesquioxane gels during aging process. Spectroscopic measurements carried out on these materials suggest the emergence of new modes of aggregation between NDI centers. Furthermore, the observation of drastic color changes from yellow to red during the aging period is attributed to the existence of redox reactions, to the formation of extended π-systems (polymorphs) and/or CT complexes.

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Poster

A new growth process for crystalline ultra-thin layers of conjugated oligomers used in field-effect transistor applications

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Abstract:

Most organic semiconductor materials dewet on silicon wafers with thermal oxide layers. While Si-wafers represent convenient substrates for building a field effect transistor (FET), dewetting largely destroys the possibility for obtaining a compact and continuous crystalline thin organic semiconductor film and thus limits the mobility in these systems. Using oligothiophenes, we present an approach where the initial dewetting process can be turned into an advantage for generating very thin but large crystalline domains of a size up to the millimetres with all molecules sharing a single orientation[1]. Our approach can be easily extended to other molecules, which have strongly differing growth velocities in the various directions of the crystal, for example due to directional π-stacking interactions. FETs devices based on such large crystalline domains showed charge carrier mobility's that were two orders of magnitude higher compared to non-crystallized films(figure 1).

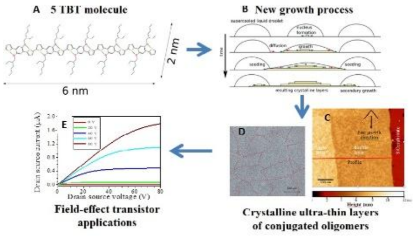

Figure 1 : From the 5TBT molecule(A) to the FET application(E) through the formation of a well-crystallized ultra-thin organic layer characterized by light microscopy(D) and AFM(C), using a new growth mechanism(B)

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Poster

Fluorescence switches based on host/guest interactions: from surfaces to hybrid supramolecular/plasmonic nanostructures

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Since many years, efforts have been made in the design of stimuli-responsive materials for different analytical and biological applications. One of the strategies developed takes advantage of the stimuli-responsive supramolecular interactions between β-cyclodextrin (β-CD) and its guests such as ferrocene (Fc) to achieve controllable surface binding.

This strategy allows to trigger electrochemically the adsorption and the release of polymers on self-assembled monolayers (SAMs) [1]. Several levels of control are achievable thanks to supramolecular interactions such as reversibility under electrochemical stimulus, strong binding due to multivalency and high selectivity [1,2]. The strategy was also applied to bifunctional linkers (Fc-biotin) to give access to biospecific and reversible immobilization of biomolecules. [3] Finally, the strategy has been extended to the capture and the release of cells using the combination of RGD ligand and β-CD/Fc redox switchable system [4].

The goal of this project is to extend this strategy from surfaces onto nanostructures such as gold nanoparticles or patterned nanoarchitectures. We propose to use fluorescent probes in combination with host/guest moieties co-immobilized on the same surface to develop hybrid supramolecular/plasmonic switches (Figure 1). By taking advantages of stimuli responsive host/guest interactions as well as strong dependence of fluorescence on the fluorophore/particle distance, we aim to achieve wide and reversible fluorescence modulation. The developed switches have potential applications as renewable sensors and multifunctional nanoprobes.

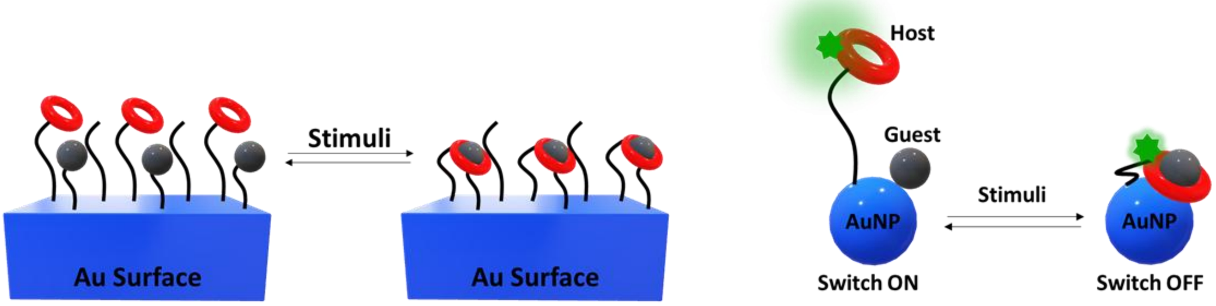

Figure 1: Host/guest chemistry: from functional surfaces to multifunctional nanostructures

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Poster

2D array of host-guest complexes as single molecule devices.

Enrique Escorihuela,[1,2] Santiago Martín,[1,2,3] Pilar Cea,[1,2,3] Ignacio Gascón,[1,2] Jesús del Barrio[1,4], Ross J. Davidson,[5] Andrew Beeby,[5] Paul J. Low[6]

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Abstract:

Nowadays, there is a significant interest in shrinking electrical devices beyond traditional complementary metal-oxide-semiconductor (CMOS) technologies by fabricating unimolecular electronic devices.[1] Moreover, one of the long-standing challenges in single-molecule electronics is controlling the precise geometry, which can dominate the performance of single-molecule devices. In this context, control of the spatial distribution and orientation of the functional compounds in extended assemblies is of utmost importance.[2] Host-guest complexes stand out for being a popular strategy for the fabrication and functionalization of new materials through non-covalent bonds. These supramolecular interactions can influence the electronic properties of the compounds that integrate the complex; as it has been observed in host–guest supramolecular interactions between a cucurbit[8]uril (CB[8]) and viologen molecular bridges.[3] Herein, we show the fabrication and characterization of a compact self-assembled monolayer formed by host-guest complexes of a viologen molecular bridge and cucurbit[7]uril, arranged in a 2D array fashion onto a gold electrode (Figure 1). Gold nanoparticles were *in situ* synthesized and deposited over the SA as the top-contact electrode. The electrical properties of these host-guest complexes are in agreement with single-molecule measurements. Therefore, this strategy allows building a large 2D array of host-guest single-molecule devices with various possible advantages, such as avoiding in-plane electron transport, large accessibility for a great variety of compounds and presents available local volume at the host cavity for electromechanically induce configurational modifications of the guest molecule.

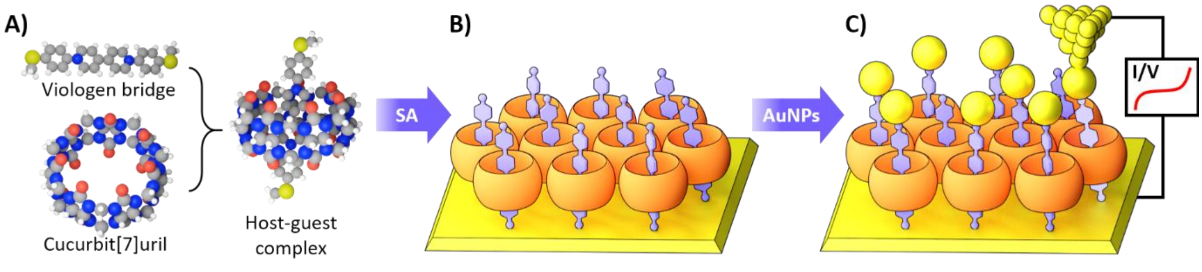

Figure 1. Scheme of the host-guest complex formation (A), monolayer self-assembly (B) and electrical measurement of the molecular array structure (C).

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Poster

Hierarchical patterning: sub-10 µm 3D structures nano-textured by block copolymer self-assembly

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Abstract:

For several years, advances in lithography have focused on reducing the size of patterns, mainly in the microelectronics sector. Today, researchers are interested in the achievement of structures combining a micrometric shape overlaid with nanostructures. These hierarchical structures have been intensively explored to mimic the properties found in nature, and more particularly on structures inspired by moth eyes. Their eyes are composed of a hexagonal array of microlens called ommatidia focus the light on the internal photoreceptors, and the surface of each lens is textured into subwavelength antireflective (AR) nanostructures. The nanopillars produce a gradual transition in refractive index at the lens interface. This reduces light reflection, thereby improving the light sensitivity of moth eyes. The AR nanostructures combined with the ommatidia arrays provide an unparalleled ability to see even in the dark and also maintain unobstructed vision in any environment thanks to super hydrophobicity. This is why numerous studies seek to mimic or are inspired by this structure. The first approaches reported in the literature to fabricate these hierarchical structures were to use the eye of a moth as a biological mold [2]. Unfortunately, this approach is severely limited by the small surface area offered by an ommatidia array and the fixed diameter / bending angle of microlens (diameter ≈ 25 µm). Several researchers have successfully patterned this hierarchical microlens structures with lithography and/or etching techniques [3]. Previously published studies are limited to lens with a diameter of more than ten micrometers. However, the measurements of the optical properties confirm the expectations towards the moth's eye, with a reduction in reflectance (Figure 1), which allows improved the light sensitivity of the imaging devices [4].

Herein, we introduce a simple and low-cost method for the manufacturing of sub-10 µm 3D structure arrays (lens or bowl) nano-textured with patterns of contacts or lines (Figure 2). A grayscale lithography process (300 mm) allows the manufacturing of 3D microstructures of different dimensions and shapes. This method aims at modulating light intensity transmittance of a photolithographic mask in order to locally control the dose received by the resist. Being non-uniformly exposed, the final shape of the resist after development can be controlled in order to produce 3D patterns [5]. Then, the nanostructures are achieved by self-assembly of block copolymers. This low-cost technique allows the achievement of cylindrical or lamellar patterns of a few nanometers period by spin-coating [6].

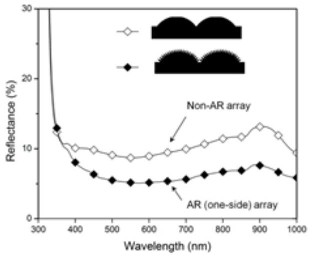

Figure 1: Multiscale ommatidial arrays with AR nanostructures versus the non-AR ommatidial arrays [4].

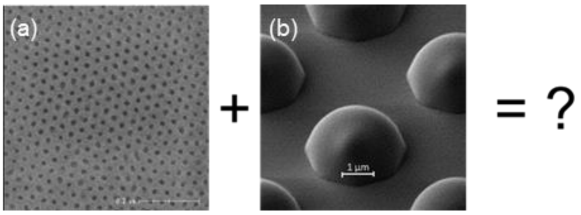

Figure 2: (a) SEM image of nanocylinders (holes) achieved by DSA (scale 0.2 µm). (b) Tiled SEM image of microlens by grayscale lithography process (scale 1 µm).

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Poster

The Substituent Touch upon the Coordination Chemistry of Diamino-benzoquinonediimines

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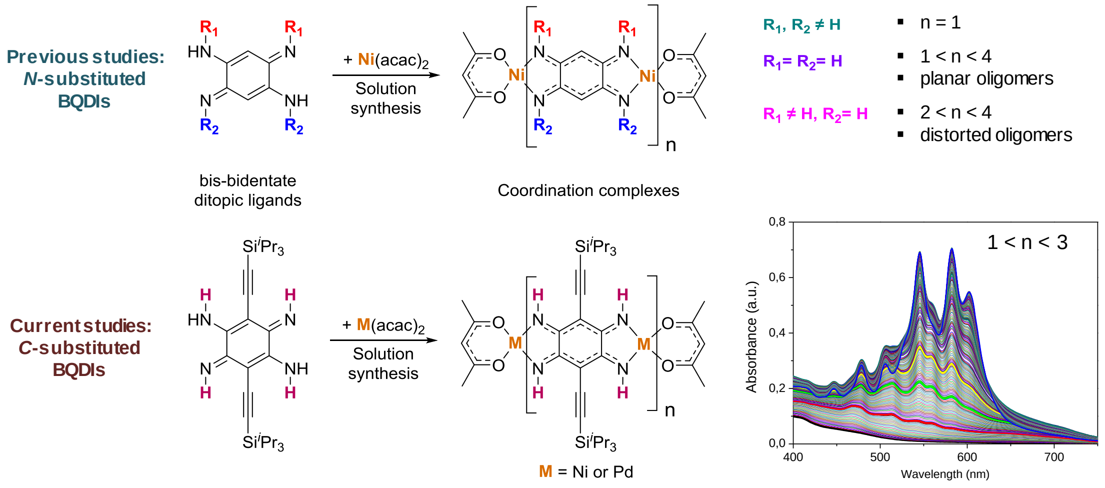
Abstract:

In materials science, a particular attention has lately been given to the development of visible and near-infrared (NIR) absorbing molecules as a response to the interest coming from optoelectronic applications.[1-2] As such, coordination chemistry enters the game with a strategy centered on solid-phase or in-solution metal-ligand assembly to reach extended or highly conjugated architectures.[3-4] In this context, 2,5-diamino-1,4-benzoquinonediimine (BQDI) stands as versatile ditopic and bis-bidentate ligand for the preparation of coordination complexes featuring catalytic, optical or magnetic properties.[5]

The complexation of such a ligand in solution is a stepwise mechanism that allows the isolation of stable mono-, di- or polynuclear oligomers with absorption up to the NIR region.[5-7] The *N*-substitution of BQDI plays an important role on the coordination properties of this building block but can notably be detrimental for the electronic delocalization between the metal centers.[7] Consequently, our present investigation takes the process one step further, by introducing *C*-substituents on the ligand and screening the metalation mechanism and optical properties of unprecedented nickel and palladium coordination oligomers.



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Poster

Structural and electrical properties of self-assembled monolayers on Ge as passivating and insulating layers

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Abstract:

Due to its high intrinsic mobility, germanium is emerging as a likely alternative material to replace silicon in the next generation of high-mobility and high-frequency field effect transistors. However, the preparation of an interfacial layer enabling to passivate and insulate Ge surface is still problematic. A promising approach consists in designing new self-assembled molecular monolayers (SAMs) [1] grafted on Ge exhibiting highly insulating and passivating properties as new high-K self-assembled nanodielectrics [2]. We have studied SAMs of model molecules such as alkylthiols and fluoro-alkylthiols, and of specially synthesized non-charged novel push-pull chromophores bearing electron donor and acceptor groups, separated by a pi-conjugated bithiophene bridge which promotes electron transfer and a subsequent dipole formation [3]. Indeed, due to the alignment of the oriented dipoles promoted by the SAM deposition strategy, such push-pull chromophores have been shown to form highly polarizable insulating films in the literature [2]. We have adapted and developed the original Ge deoxidation/grafting technique in hydro-alcoholic solution [4] and shown that, compared to the usual deoxidizing acid treatment, it gives smoother surfaces and well-organized SAMs, which is proven by ellipsometry, wettability, and scanning probe microscopy analyses. The grafting of alkylthiols and fluoro-alkylthiols on Ge has been performed directly in a single step, whereas for the push-pull chromophores designed with a carboxylic anchoring group, we have achieved a two-step grafting with amide bonding on pre-assembled amine-terminated sticking layers. Among the latter, we have demonstrated aminothiophenol SAMs exhibit a better arrangement than cysteamine, with a smooth monolayer film suitable for grafting ordered push-pull SAMs on top. UV-Visible absorption spectroscopy of push-pull chromophores in solution was used to determine the concentration limit to avoid aggregation. X-ray photoelectron spectroscopy (XPS) and infrared spectroscopy (FTIR) analyses demonstrate the oxide removal from the Ge surface after the SAM formation. Statistical electrical analyses revealed that with such push-pull SAMs, we have been able to decrease the current by a factor of 10^5 compared to Ge, and 10^4 compared to dodecane SAMs of similar thickness. Results have been analyzed by transition voltage spectroscopy [5], and successfully correlated with spectroscopic analyses of molecular levels, using inverse photoemission spectroscopy and XPS valence band determination for probing the unoccupied and occupied molecular orbitals respectively, as well as with DFT calculations, thus allowing to identify the highest occupied molecular orbital as the level involved in the electronic transport through the push-pull SAM. Dipole formation has also been evidenced in the SAM.

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Poster

Derivatives of diarylethene (DAE) as functional molecular building blocks to build an Electrocatalytic Self-assembled system for the oxygen reduction reaction.

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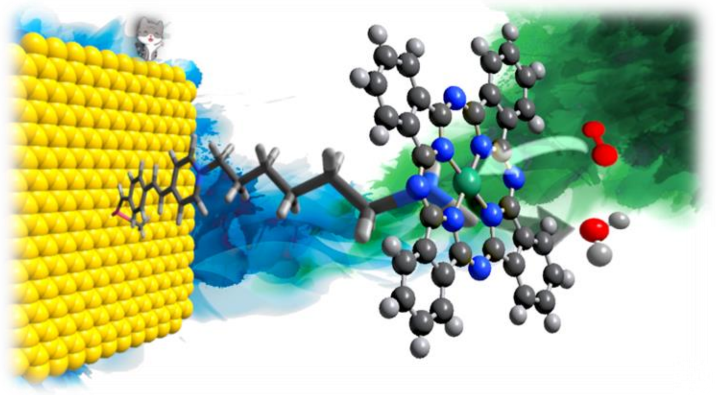
The oxygen reduction reaction (ORR) is one of the most important reactions in electrochemistry as it is involved in energy conversion systems, such as fuel cells.[1,2] ORR at room temperature is a spontaneous process in a H_2/O_2 fuel cell, however, its kinetics in most electrodic materials is slow and requires the use of catalysts.[2] Among the alternative electrode materials that have emerged to catalyze ORR is the electrode surfaces, modified with **catalysts of MN4 complexes such as iron phthalocyanines, FePc.** An example of this is the **self-assembled FePc systems on gold surfaces**,[3] Fig. 1. In these systems, the construction is carried out by modifying an electrode surface, with self-assembled organic monolayers (SAMs) and their subsequent functionalization with FePc, forming an "umbrella" type configuration.[3] In these systems, the SAMs molecules (**molecular building blocks**) act as: (i) **axial ligand** in FePc, fulfilling the role of slightly uncoupling the active site (metal center) from the surface and (ii) **as molecular wires** allowing transport electronic between the electrode surface and catalyst Fig. 1. In search of "**molecular building blocks**" for the development of nanostructured devices for RRO, **SAMs** formed from **derivatives of diarylethene (DAE)** are excellent entities due to their structural properties that give them **interesting charge transfer processes** (CT). Thus, this research work corresponds to the first stage of construction and characterization of self-assembling FePc systems based on DAE SAMs functionalized with FePc on Au (111) surfaces. For this, the **"bottom-up"** construction strategy was used.[3] The molecular building blocks DAE (diarylteneum Pyridinium, 1- (3-aminoethyl) -4- [2- (4-thiophenyl) ethenyl] -2,2,2-trifluoroacetate) were rationally designed and synthesized to anchor to a surface gold on one end and coordinate FePc on the other. The self-assembling system was characterized electrochemically using cyclic voltammetry, square wave (LSV), and tunnel-break junction microscopy (STM-BJ).



Au / (DAE) / FePc self-assembled system scheme for ORR.

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Poster

Chirality from scratch: enantioselective adsorption in geometrically controlled lateral nanoconfinement

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Abstract:

Understanding enantiospecific interactions is crucial for the development of many research areas, such as chiral separation techniques, enantioselective heterogeneous catalysis[1] and chiral functional materials in general.[2] Visualizing chirality at interfaces provides valuable insights into these processes. For this, scanning tunnelling microscopy (STM) is a suitable technique as it can provide sub-molecular resolution of enantiospecific interactions by imaging 2D self-assembled chiral structures.[3]

In this work, chiral symmetry breaking in molecular adsorption at the solid/liquid interface is obtained by using lateral geometric nanoconfinement. Such chiral nanoconfinement is created at the interface of achiral covalently modified highly-oriented pyrolytic graphite (HOPG) and a racemic solution by *in situ* scanning probe lithography (Figure 1). Our results show that enantioselective adsorption of chiral molecules can be achieved by adjusting the relative orientation between the nanoconfining walls and substrate symmetry direction.[4] With this method, the adsorption of the selected enantiomer is more than six times higher compared to the mirror image molecule. This approach can provide new insight into the process of recognition and selection of chiral molecules, in particular kinetic and thermodynamic aspects can be unravelled.

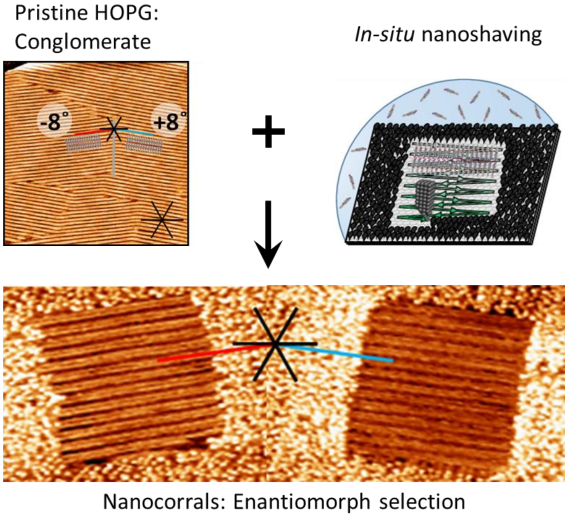

Figure 1. The self-assembly of a racemic mixture at the HOPG/liquid interface is combined with a nanoconfined environment. This combination enables preferential adsorption of targeted chiral structures formed by one desired enantiomer contained in the racemic mixture. Thus, chiral separation can be achieved.

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Poster

Unravelling the growth mechanism of (3,1) graphene nanoribbons on a Cu(111) surface

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Abstract:

Graphene nanoribbons (GNRs) are 1D graphene stripes which are widely investigated due to their remarkable electronic properties compared to 2D graphene. To achieve GNRs with well-defined edge configuration and width, and accordingly control these electronic properties, growth was performed from wisely-chosen molecular building-blocks and was optimized thanks to atomic-scale characterizations using scanning probe microscopies under ultra-high vacuum (UHV). Non-halogenated 9,9'-bianthryl derivatives lead to chiral (3,1)-GNRs, but only on a copper surface. After few controversies, the currently accepted reactional mechanism for the growth of chiral (3,1)-GNRs on a Cu(111) surface is based on a first thermal annealing leading to a protopolymer thanks to on surface-assisted generation of a 2,2'-diradical species. [1] Then, further heating gives the targeted chiral (3,1)-GNR as result of ring-closure driven by a cyclodehydrogenation. Most of the reaction intermediates involved in this mechanism have been observed. Here, we investigate the growth of laterally functionalized (3,1) chiral GNRs by thermal-induced reaction of 10,10'-di(aryl)-9,9'-bianthryl on a Cu(111) surface underUHV by scanning tunnelling microscopy (STM). We find that the growth of GNRs is not possible when the 10,10' positions of the starting building blocks are substituted by aryl groups. Therefore, we revisit the commonly accepted reaction mechanism accounting for the growth of (3,1) GNR on a Cu(111) surface to explain this phenomenon. [2]

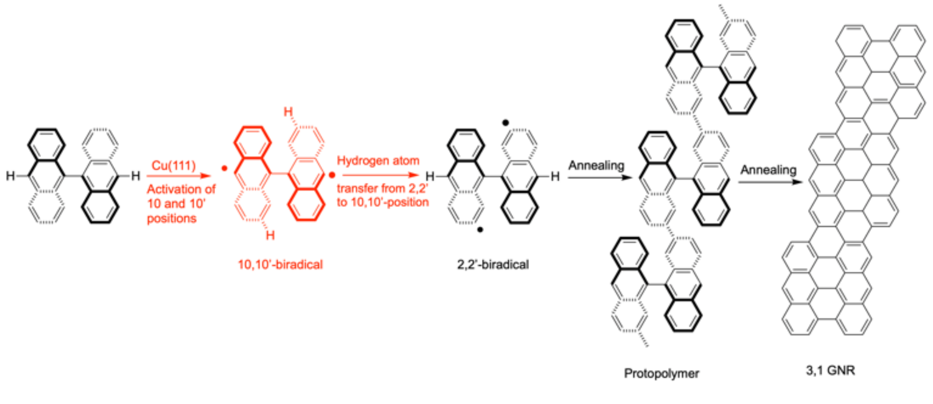

Figure: Completed reaction mechanism for the growth of (3,1) GNR induced by a two-step annealing of BA molecules on a Cu(111) surface. The formation of 10,10'-biradical (in red), followed by radical transposition, is added as initial step.

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Poster

On surface synthesis of Por-GNRs on Au(111) and exploration of a new path to decouple molecules from a metallic support

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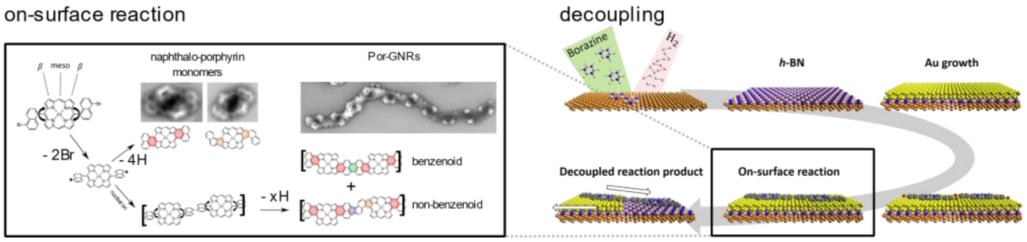
Abstract:

In recent years, the on-surface formation of hybrid structures combining porphyrins (Pors) and graphene nanoribbons (GNRs) attracted increasing interest due to their potential for electronic, optoelectronic and spintronic applications [1-3]. Control of the precise atomic structure of such covalently linked porphyrin-based heterosystems is highly relevant for the tuning of their electronic and functional properties. Examples achieving high yields in combination with selectivity are still scarce [2,4]. Here, we report the on-surface synthesis of extended benzenoid and non-benzenoid coupled porphyrin-graphene nanoribbon hybrids (Por-GNRs) by sequential Ullmann reaction and cyclodehydrogenation of the Zn(II) 5,15-Bis(5-bromo-1-naphthyl)porphyrin (Naph-Por) precursor on Au(111). Through bond-resolved non-contact atomic force microscopy (nc-AFM) and scanning tunneling microscopy (STM) the reaction is characterized in detail and insight into the effect of temperature and the annealing protocol is obtained.

A major drawback of on-surface synthesis on noble metal surfaces, performed as described above, is the influence of the substrate on the intrinsic properties of the reaction product. A common way to reduce detrimental adsorbate-metal interactions is to place the reaction product onto an insulating thin film by STM tip-manipulation. This procedure, however, is very tedious. Here, we explore a different approach to obtain the reaction product on an insulating layer, avoiding tip-manipulation, while still being able to exploit established on-surface synthesis procedures. Extended fcc(111) terminated Au islands (typical lateral extension 10 – 20 nm) are grown on *h*-BN/Cu(111) serving as catalyst for the on-surface reaction. Through annealing, migration of the reaction product onto the insulating *h*-BN layer is induced. Even though we can only achieve low yields of Por-GNRs and of covalent TBB structures on *h*-BN so far, further optimization of the process might open pathways towards a general protocol to decouple molecules.



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Poster

The effect of I^- addition to the stability of Cd(0001) electrode | RTIL interface

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Abstract:

Since the discovery of moisture-resistant ionic liquids (ILs), they have been in the focus of numerous studies due to their unique properties and a vast number of potential applications. For example, the large electrochemical stability of ILs makes them attractive electrolytes for energy storage devices such as supercapacitors and batteries [1]. In supercapacitors, the energy is stored at the electrode | electrolyte interface. One way to improve the capacitance of the metal | IL interface is to add specifically adsorbing halide ions to the electrolyte. Previously, it has been shown by Siimenson and Siinor *et al*. [2,3] that the Bi(111) electrode interfaces with mixtures of $EMImBF_4$ and EMImI have significantly higher capacitance than pure $EMImBF_4$ while maintaining reversibility and time-stability. As the electrodeposition of Cd has been used in the production of electronic devices, assessing the processes occurring at the Cd | IL interface is essential in the design of further applications.

In this study, we have investigated $EMImBF_4$ mixtures with EMImI addition using electrochemical impedance spectroscopy, *in situ* scanning tunnelling microscopy (STM), and density functional theory (DFT) calculations to determine the electrochemical properties of Cd(0001) | IL mixture interface in the case of larger halide ion concentration. The specific adsorption of I^- along with partial charge transfer, increased the interfacial capacitance considerably. At the same time, the interface was determined to be unstable in time, as the interfacial capacitance and electrode's surface roughness increased over 72 hours. This trend we related to the dissolution of the Cd(0001) surface, which is induced by the addition of I^- that forms more stable complexes with Cd^{2+} than BF_4^- ions.

Acknowledgements:

This work was supported by the Estonian Research Council grant PSG249, by the Archimedes Foundation under project TK141 "Advanced materials and high-technology devices for sustainable energetics, sensorics and nanoelectronics", and by University of Tartu ASTRA project PER ASPERA through Graduate School of Functional Materials and Technologies (GSFMT).

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Poster

Behavior of an Azobenzene Derivative on Gold Exposed to Ultraviolet Light or Electric Field

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In recent years, molecular switches such as azobenzene adsorbed on metal surfaces have attracted considerable attention due to their potential use in nanotechnology, information storage or molecular electronics[1,2]. In particular, the 3,3',5,5'-tetra-tert-butylazobenzene (TBA) molecule is a promising candidate for such studies, due to the four lateral tert-butyl-groups which act as "spacer leg" to reduce the electronic coupling between the active part of the molecule (azobenzene) and the metal surface. This azobenzene derivative switches reversibly between the two isomeric states (*trans*-TBA and *cis*-TBA; Fig. 1a). This isomerization has already been demonstrated by STM using either the electric field induced by the STM tip[3] or by exposure to UV or blue light[4].

Here we report a comparison between the effect of electric field and UV light exposure at 305 nm on TBA deposited on Au(111) surface, investigated by low temperature STM (77K or 4K). After the TBA evaporation, molecules are organized on the gold surface and appear in the *trans* isomer with four lobes corresponding to the 4 "legs", with an apparent height of 0.25 ± 0.02 nm (Fig. 1b). By STM imaging at -2V (Fig. 1c), bright spots appear in the middle of some TBA molecules, with an apparent height of 0.36 ± 0.05 nm (Fig. 1d bottom). These spots are usually associated to the *cis*-TBA and induced by the *trans*-TBA to *cis*-TBA isomerization under the presence of an electric field[3]. However during STM imaging at -2V, these spots blink (Fig. 2d top), suggesting here a isomerization of the TBA molecule also from *cis* to *trans*. In the case of UV exposure, we observe also systematically a modification of the *trans*-TBA arrangement with the apparition of linear structures spaced at about 450 pm (Fig. 1e). The origin of these structures induced by UV on *trans*-TBA molecules will be discussed.

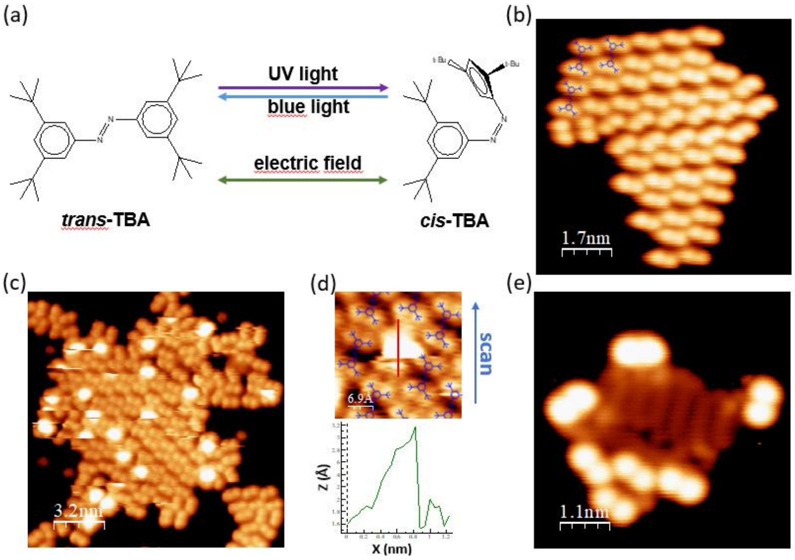

Figure 1: Isomerization of the TBA molecule with light or electric field between the two isomers *trans*-TBA and *cis*-TBA (a); STM constant-current image 8.7 x 8.7 nm² of TBA after deposition on Au(111), V = + 1.5 V, I = 20 pA (b); STM image 16.1 x 16.1 nm² of TBA at V = - 2 V, I = 5 pA (c); zoom 3.5 x 3.5 nm² from (c) on a bright spot with the corresponding profile in bottom (d); STM images 5.7 x 5.7 nm² of TBA after UV exposure at 302 nm during 12 h and with an intensity of 0.5 mW/cm², V = - 1.5 V, I = 5 pA (e).

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Poster

The roles of atomic hydrogen in on-surface synthesis unraveled by in-situ ToF-SIMS

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Abstract:

Atomic hydrogen is a side product of many chemical reactions in on-surface synthesis that was expected to simply desorb without consequences. Here, different aspects of transient atomic H at surfaces, showing a more complex reality, are illuminated.

The results are based primarily on *in-situ* time-of-flight secondary ion mass spectrometry (ToF-SIMS), a unique approach that is ideally suited to study on-surface polymerization, dehydrogenation and hydrogenation reactions in large molecules up to ~4000 u.

In combination with other surface analytical tools, the kinetics of atomic H in the desorption of Br as HBr in consequence to forming a C-C bond formation by cyclodehydrogenation is deciphered.[1] It is also shown that atomic H cleaves C-C bonds in geodesic polycyclic aromatic hydrocarbons.[2] This reaction is the exact opposite to the cyclodehydrogenation reaction. Finally, by H/D isotope exchange the dynamic nature of hydrogen in molecules at hot metal surfaces is demonstrated.[3]

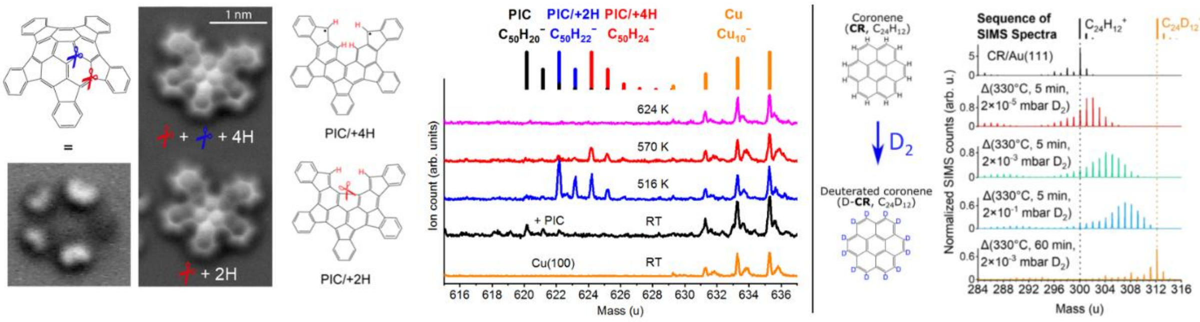

Figure 1: (Left) Hydrogenation and C-C bond cleavage in pentaindenocorannulene on Cu(100) studied by non-contact atomic force microscopy and ToF-SIMS. (Right) H/D isotope exchange in coronene on Au(111) revealed by ToF-SIMS.

References:

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Poster

Electronic Absorption Spectra Of Platinum (II) Complexes Used For Sensitized Solar Cells: DFT/TDDFT Study

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Abstract:

Using the time dependent density functional theory (TD-DFT), we studied in this work the electronic absorption spectra of a series of heteroleptic complexes using ferrocene based dithiocarbamate complexes involving Pt(II) in the form [M(dppf)L] [where dppf =1,10-bis(diphenylphosphino)ferrocene, M=Pt(II) and L= p-tolylsulfonyl dithiocarbimate, p-$CH_3C_6H_4SO_2NCS_2$ **(1)**. M=Pt and L= p-chlorobenzene sulfonyl dithiocarbimate, p-$ClC_6H_4SO_2NCS_2$ **(2)**. M=Pt and L= p-bromobenzene sulfonyl dithiocarbimate, p-$BrC_6H_4SO_2NCS_2$ **(3)**. These complexes have been synthesized and characterized experimentally using the spectroscopy methods (IR, ^1H, ^{13}C and ^{31}P NMR and UV-Vis) and crystal X-ray diffraction[1]. Due to their photo-physical and photo-chemical properties, they have been used as photosensibilisator in the DSSC (Dye Sensitized Cell Solar). For each complex our contribution was made in two main steps. The first is a geometry optimization to find the optimal structure with the density functional theory (DFT). We using the CAM-B3LYP density functional and B3LYP, using 6-31G (d,p) and 6-31G+(d) basis as implemented in Gaussian09. The study of HOMO, LUMO has been used to explicate information about charge transfer in molecules. Lastly, from the frontier molecular orbitals we elucidate the UV-vis spectra and electronic absorption proprieties. The calculated spectrums have been compared with the experimental result[2]. We have chosen to improve the efficacy of the dye in DSSC by introducing an anchor ligand –COOH with a thiophen auxiliary group in M(dppf) NCS_2 (M=Pt(II)), and substitute the ligand L=p-$XC_6H_4SO_2$ (X=CH_3, Cl, Br) with 2-Thiophene carboxylic acid which has a hypsochrome effect on the absorption spectrum due to the π-conjugation and the strong auxochrome resulting from the thiophene.

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Poster

Attenuation Factors in Molecular Electronics: Some Theoretical Concepts

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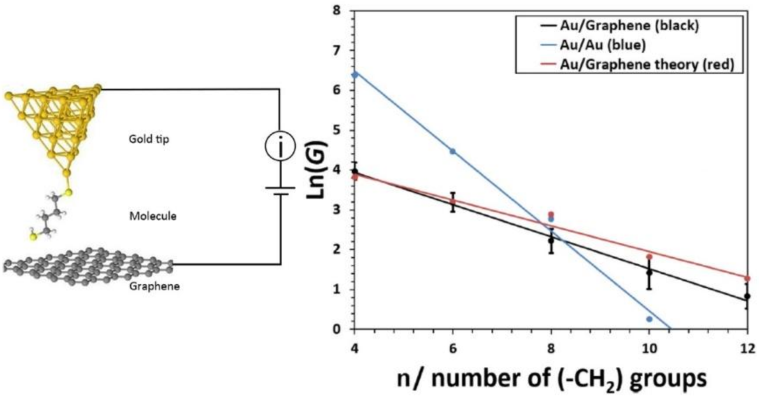
Abstract:

One of the main goals of molecular electronics is to mimic standard electronic circuits using molecules instead of p-n junctions like components based on silicon. To do so, the first property to achieve in a molecular junction is to favor and understand at the fundamental level the circulation of the electronic current through the molecule. Hence, understanding the electronic transport mechanisms in molecular junctions is of paramount importance to design molecular devices and circuits. The problem of the electronic conduction mechanism in a molecule connected to metallic electrodes is very complex. In particular, the role of the different junction components contributing to the current decay—namely the attenuation factor—is yet to be clarified. In this presentation, I will discuss the main theoretical approaches to tackle this question in the non-resonant tunneling regime. I will illustrate my purpose through standard symmetric junctions and through recent studies on hybrid molecular junctions using graphene electrodes. In each case, I will try to highlight the contribution from the anchoring groups, the molecular backbone and the electrodes, respectively. In this respect, I will consider different anchoring groups and asymmetric junctions. Finally, in light of these results, I will discuss some perspectives to describe accurately the attenuation factors in molecular electronics.



(Left) *Schematic representation of the hybrid metal–molecule junction formed in the experiment for conductance measurements.* ***(Right)*** *Evolution of the conductance as a function of the molecular length: experimental measurements on asymmetric metal–graphene junction (black), experimental measurements on symmetric metal–metal junction (blue) and conductance calculation on asymmetric metal–graphene junction (red).*

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Poster

Towards ab-initio accuracy on predicting optical band for organic crystals

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Abstract:

Recently we proposed a model Hamiltonian method that works for huge aggregated system, which represents the quality of an ab-initio excited state method, i.e. TDDFT, CC2, ADC(2). The main idea is by using a diabatization scheme[1] to capture the site energies and the corresponding couplings of dimers in the aggregated system, and then merge these elements into a "complete" coupling matrix for the aggregated system. Followed by a simple diagonalization, we could get the excitation energy of the whole aggregated system at the quality of the used ab-initio excited state method, while the computational cost is greatly reduced. The method can also be served in different level of accuracy.

We have first tested few sample systems, from thiophene tetramer to Y6 trimer to compare with the full QM results and both results are in a very good agreement. We have also formed a Y6 aggregate of 38 Y6 monomers (3230 atoms) from an optimized Y6 crystal structure[2], and predicted the corresponding optical band. The calculated excitation energy of the Y6 aggregate has been brought down from 2.1 eV to 1.8 eV, which is about 0.3 eV lower than the ones of a Y6 monomer. Although the calculated optical band is still 0.4eV higher than the measured value, we believe by applying a higher level of accuracy calculation, the calculated excitation energy will be further close to the experimental value of the Y6 crystal.

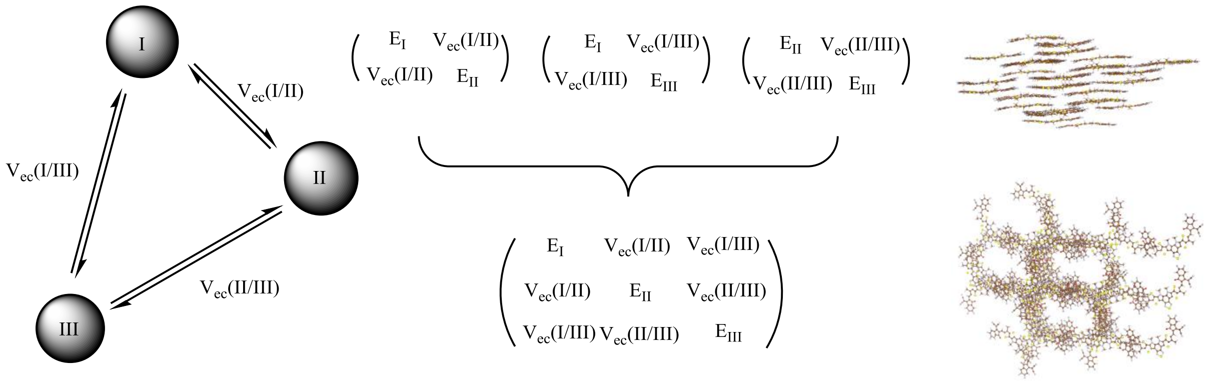

Figure 1. Left : a simple trimer interaction scheme; middle: merging dimers' coupling matrices into a trimer's coupling matrix; right : side view(up) and top view(down) of the calculated Y6 aggregate.

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Poster

Charge-transfer chemical reactions in nanofluidic Fabry-Pérot cavities

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Abstract:

We investigate the chemical reactivity of molecular populations confined inside a nanofluidic Fabry-Pérot cavity[1] (see Figure 1). Due to strong light-matter interactions developing between a resonant electromagnetic cavity-mode and the electric dipole moment of the confined molecules, a polariton is formed[2]. The former gets dressed by environmental vibrational and rotational degrees of freedom of the solvent[3]. We call the resulting polariton dressed by its cloud of environmental excitation a "reacton", since it further undergoes chemical reactions. We characterize how the reacton formation modifies the kinetics of a photoisomerization chemical reaction involving an elementary charge-transfer process. We show that the reaction driving-force and reorganization energy are both modulated optically by the reactant concentration, the vacuum Rabi splitting and the detuning between the Fabry-Pérot cavity frequency and targeted electronic transition. Finally, we compute the ultrafast picosecond dynamics of the whole photochemical reaction. We predict that despite optical cavity losses and solvent-mediated non-radiative relaxation, measurable signatures of the reacton formation can be found in state-of-the-art pump-probe experiments.

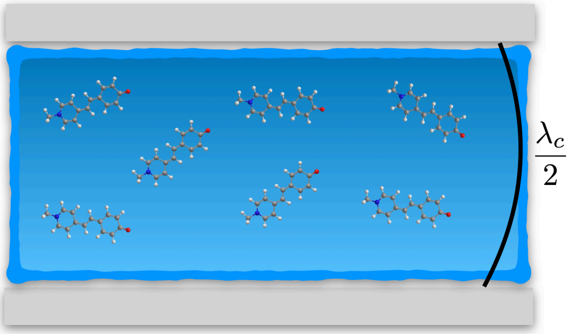

Figure 1: Pictorial representation of molecules of (E)-4-[2-(1-methylpyridin-1-ium-4-yl)vinyl]phenolate, in solution inside a nanofluidic Fabry-Pérot cavity.

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Poster

Donors, acceptors and (a bit of) aromatic:

A computational study of molecule-surface interactions onto 2D hexagonal boron nitride towards hybrid electronic interfaces

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Abstract:

Two-dimensional materials, like graphene and hexagonal boron nitride (hBN), can be employed to build innovative photochromic and optoelectronic devices to capture and convert light into energy, thanks to their unique surface physico-chemical properties [1, 2]. Indeed, it has been shown that hBN-based materials can find important applications in the design of electronic devices, thanks to its electrical insulation and efficient thermal transport capabilities. Further functionalities and specific moieties can be also introduced, generating so-called “hybrid organic / inorganic surfaces” (HIOS), whose architecture is based on non-covalent interactions, i.e. van der Waals (vdW) dispersion forces [3, 4]. Here, we aim at computationally investigate and design nanostructured systems based on hBN and organic chromophores [5, 6]. Specifically, we look at interfaces formed after the adsorption of prototypical organic structures, ranging from simple aromatic hydrocarbon (pyrene) to heterocyclic compounds used as n-type and p-type dopants used in organic electronics like tetracyanoquinodimethane (TCNQ) and tetrathiafulvalene (TTF), onto free-standing 2D hBN by means of periodic density functional theory calculations. Through an accurate electronic structure description using vdW-corrected hybrid functionals we highlight properties of the hybrid interfaces against the isolated BN or the gas-phase molecules. According to our study, hBN can form stable structures with the adsorbates thanks to the strong $\pi - \pi$ stacking, yet maintaining its original properties. While the adsorption does not perturb the underling electronic structure of the surface, level alignment of frontier molecular orbitals with respect to the conduction (CB) and valence band (VB) edges of hBN can lead to the appearance of buried electronic states of the molecule, therefore suggesting the possibility to induce excitonic transitions between adsorbates and surface.

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Poster

New approach to the molecular electronics on the example of ethane, ethylene, benzene and acetylene

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Abstract:

Molecular electronics has been described in this research work by introducing some innovative elementary theoretical concepts such as:

- interpretation of the free electron pair not as a concentration of the electron cloud on one side of the nucleus (lone pair), but as a symmetrical distribution of the electron cloud on both sides,

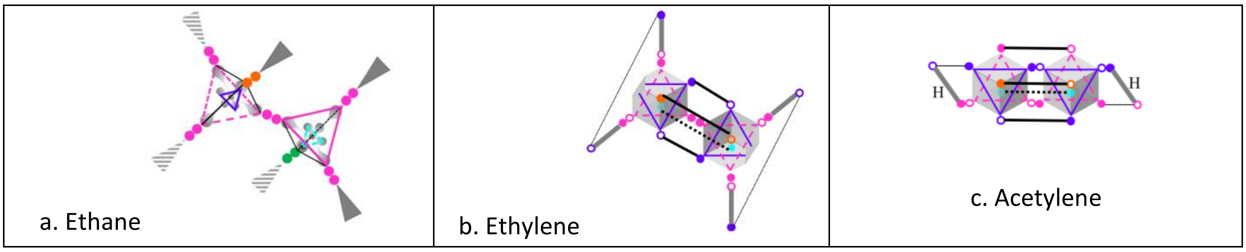
- hypothesis that in polar bonds and the vast majority of multiple bonds, one electron is shared, not an electron pair and distinction of intermolecular bonds in *bi-electronic* and *mono-electronic*,

- consideration that the formation of multiple bonds occurs thanks to the transformation of *bi electronic* bonds (sigma) into *mono-electronic* bonds ; this transformation serves to increase the quantity of electrons available to form pi bonds which intensifies the cohesion between the atoms,

- interpretation of the transformation of the geometry of molecules in relation to the number of bonds as a result of changes in the spatial relationships between atoms, and not as a result of the hybridization of orbitals and prediction and calculation of the spatial parameters of molecules (topology, bond lengths and angles) by applying trigonometric equations and other geometric rules.

This new molecular theoretical model offers new tools for interpreting different properties of molecules. For example, it is able to explain several characteristics structural and electronics of benzene and its derivatives, such as the differentiation of the spin density of the adjacent hydrogens in the ring, the differentiation between the activating and deactivating substituents of the electrophilic substitutions, the degrees of aromaticity of the condensed rings and of the annulenes.

Figure



a. Ethane

b. Ethylene

c. Acetylene

Colors indicate binding plans and single line indicates an electron of the π bond equally shared between two atoms. a) Ethane: bond length C - C ≈ (√3l) / 2 ≈ 153.20 pm, bond angles HCH ≈ 109.5^{o}. b) Ethylene: bond angles CCH ≈ 120^{o}, bond length C - C ≈ (√2l) / (√3) ≈ 141.98 pm, but the C-C bond in ethylene is not stretched in three directions which reduces its calculated value ; the calculated value is perfect in graphite and graphene.
c) Acethylene: bond length C - C ≈ (√2l) / 2 ≈ 153.20 pm, bond angles CCH ≈ 180^{o}.

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Poster

Relevance of Shockley states on the electrical response of gold-based molecular junctions

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Abstract:

Gold breaks exposing preferably (111)-oriented surfaces, that host Shockley type surface states (SSs) [1]. Nevertheless, the relevance of SSs on the electrical properties of gold-based molecular junctions has not been explored in detail. Here, we show that the gold (111) SS, that lies ~ 0,5 eV below the Fermi energy, is key to determining correctly the electrical and thermal response of the above junctions. We also show that the gold SS appears only if d-orbitals are included explicitly in the valence shell. We discuss in detail a Benzenediamine (BDA) and a Benzenedicarbonitrile (BDCN) gold (111) junction, where we also include the DFT+Σ correction scheme that overcomes some of the limitations of the generalized gradient approximation (GGA) to predict the correct electronic gap [2].

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Poster

The role of molecular packing in the optical response of small-molecule OPV materials

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Abstract:

Computational protocols for performance assessment are becoming more and more widespread as tools to explore the vast space of organic semiconductors. In molecular electronics, a small set of environment-dependent photo-physical and electrical properties are known to be relevant for most applications. The protocols are therefore faced with the task of evaluating these physical quantities, such as exciton or charge transport efficiencies, that require to include a modelling of the microscopic environment at different length scales. Here, we consider the specific case of a small-molecule photovoltaic material for which the details of molecular packing have pronounced effects on larger-scale transport properties as well as more local ones, such as optical response, due to the large susceptibility of small molecular systems to their electrostatic environment. A computational protocol developed in the group that includes a minimal modelling of the solid-state environment has been deployed to study a compound consisting of a methyl-diphenylamine donor group linked to a dicyanovinyl acceptor via a thienyl ring (MDTD), used as donor in experimental solar devices [1,2]. MDTD thin films display a marked change in absorption when subject to thermal treatment[1]. The final spectrum appears broadened and redshifted, conferring these films improved light-harvesting efficiency. Our computational approach has allowed the identification of the microscopic packing details likely responsible for this change. Different possible low-energy MDTD crystal polymorphs have been investigated and two have been found to display absorption bands reproducing well the observed ones. The first coincides with the experimentally reported bulk crystal structure[1] (H aggregates) while the other features a molecular packing with head-to-tail molecular stacking (J aggregates). The conversion between the two forms, triggered by thermal treatment, has been found to be the most plausible explanation for the reported change. By fitting the reported spectra with predicted ones, we were also able to provide an estimate for the relative proportion of the two polymorphs in the films. An indication of their relative free energy difference. In addition, a charge mobility simulation has been carried out in order to assess the impact of this morphology reorganization on transport efficiency. Simulated mobilities on the morphology inferred from absorption analysis are compatible with experimental data and provide a further validation to our findings[3].

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Poster

Local orbitals for ab-initio and many-body simulations of nanoelectronic devices

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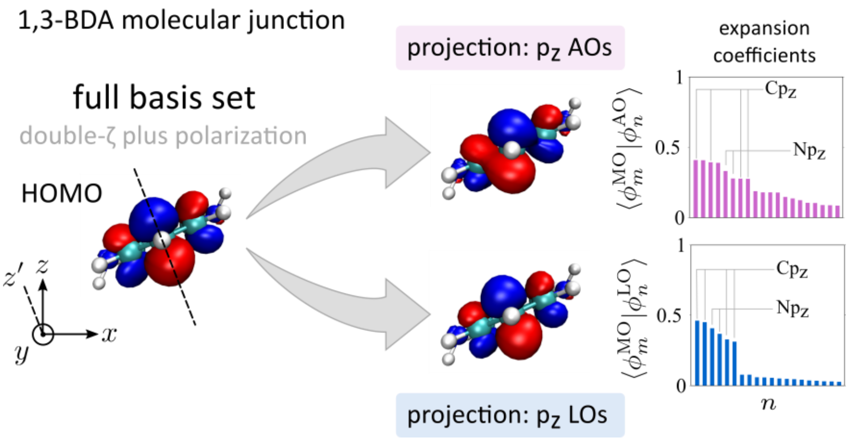
Abstract:

Atomic-like orbitals (AOs) within the LCAO formalism allow for computationally efficient calculations within density functional theory (DFT) although the numerical accuracy is limited by the quality of the basis set. At the same time, considering extensive basis sets poses a fundamental problem of physical interpretation of the results.

An alternative is to define local orbitals (LOs) which inherit the information of the local crystal field and have a natural physical interpretation. This can be done by subdiagonalization of the individual atomic blocks of the LCAO Hamiltonian. Keeping a suitable subset of relevant LOs is sufficient to provide an accurate description of the physics around the Fermi level, thus reducing to some extent the redundancy of the original basis set.

Hence, LOs allow for, e.g., efficient DFT calculations of electronic structure and trasport properties without sacrificing the numerical accuracy. Such a reduced basis set is also useful for the definition of a ab-initio effective Hamiltonians to take into account many-body effects beyond DFT.

We demonstrate the utility of LOs for materials with different chemical and physical properties, and we analyze strategies and perspectives for future applications.



Projection of a benzene-dithiol molecular junction HOMO onto a subset of atomic orbitals with p_z symmetry. As the LOs inherit information about the atomic chemical environment, they provide a better projection of the HOMO with respect to the AOs of the original LCAO basis.

References:

G. Gandus, A. Valli, D. Passerone, and R. Stadler, J. Chem. Phys. **153**, 194103 (2020)

Poster

Demonstrating Analog Resistive Switching Behaviour in Squaraine Nanowire Networks

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Abstract:

Conventional computing based on the von Neumann chip architecture will soon become outdated, with innovative materials and device architectures required to satiate the demand for faster, cheaper, more efficient electronic devices.[1] Organic nanowire (NW) networks with memristive properties are suitable candidates to help circumvent the ‘von Neumann bottleneck’. Memristors, or resistive random-access memory devices, can provide multi-level memory, and are characterised by pinched hysteretic *I-V* loops.[2] These features enable exponentially more memory to be stored per the same unit area as compared with conventional devices, as well as facilitating the co-location of memory and logic operations. In addition, the gradual changes in conductance of analog memristors has important implications for the successful implemementation of synaptic functionality in hardware.

Herein we demonstrate a self-assembled analog resistive switching NW network device displaying the memory functionality of a memristor, based on NWs of 2,4-Bis[4-(diethylamino)-2-hydroxyphenyl]squaraine (SQ), a small-molecule organic semiconductor. The device shows gradual changes in conductance (rather than abrupt), and hence does not require an electroforming step. We postulate that charge trapping, an almost ubiquitous phenomenon in rapidly self-assembled nanostructures,[3] is responsible for the inherent memory functionality. The small grain size in the NWs (compared with their diameter) lend the charge trapping hypothesis credibility, as well the presence of a single partial semicircle in the Nyquist plot following AC impedance measurements under illumination, making the presence of ions unlikely. SQ, being a p-type semiconductor, and also allowing for the offset between the LUMO of the NWs and the Fermi level of the Au electrodes, lends itself to ‘hole-only’ transport in this case, helping to explain the symmetrical nature of the hysteresis loops in the positive and negative bias directions. From analysis of the *I-V* measurements, Ohmic and space-charge-limited (SCL) conduction are seen to be the dominant conduction regimes present. The device demonstrates excellent stability and write endurance (~10^3-10^4 write pulses without sign of degradation), the latter being a key requirement for online learning, otherwise known as learning on-the-fly. In addition to this, the memory retention lasts beyond a couple of minutes which is also satisfactory for online learning applications where the synaptic weight values can be stored elsewhere following the training process.[4] Furthermore, the device is also responsive to visible light excitation which opens the door to the possibility of novel device functionality such as photonic memory. NW networks based on SQ possess properties that may enable embedding of memristive circuits in hardware.

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Poster

Synthesis of new photo-generated diazonia derivatives as potential DNA intercalating agents

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Abstract:

Recently, an intramolecular double nucleophilic aromatic substitution (S_NAr) has been discovered for the development of an anti-cancer treatment by stabilizing selectively the G-quadruplexes structures.[1] Photo-conversion of **1** into a diazonia **2** stands for an innovative alternative to cancer treatments by causing cell death in a non-invasive way using light. From our knowledge, the mechanism of such an intramolecular double S_NAr has never been reported.

Here, we present an electrochemical approach aiming at elucidating the reaction mechanism by characterizing the involved intermediate Meisenheimer complex (σ^H- or σ^X-complexes).[2] Moreover, cyclic voltammetry experiments allow us to compare and rationalize the oxidative potentials and kinetics depending on the leaving group which has been chosen as a halogen or a triflate.

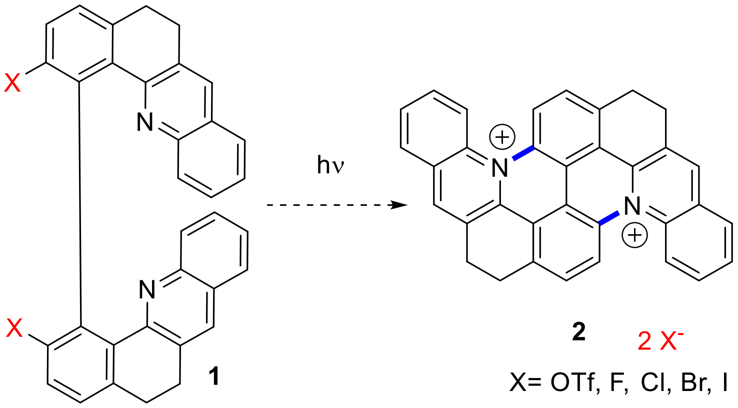

Figure 1 – Quinolizinium derivatives photoconversion into a diazonia.

References:

1. Deiana, M. *et al.* Light-induced in situ chemical activation of a fluorescent probe for monitoring intracellular G-quadruplex structures. *Nanoscale* **13**, 13795–13808 (2021).
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Poster

An Electronic Nose with one Single Conducting Polymer? How Mild-Doping Tunes P3HT's Chemo-Sensitivity for Molecular Recognition

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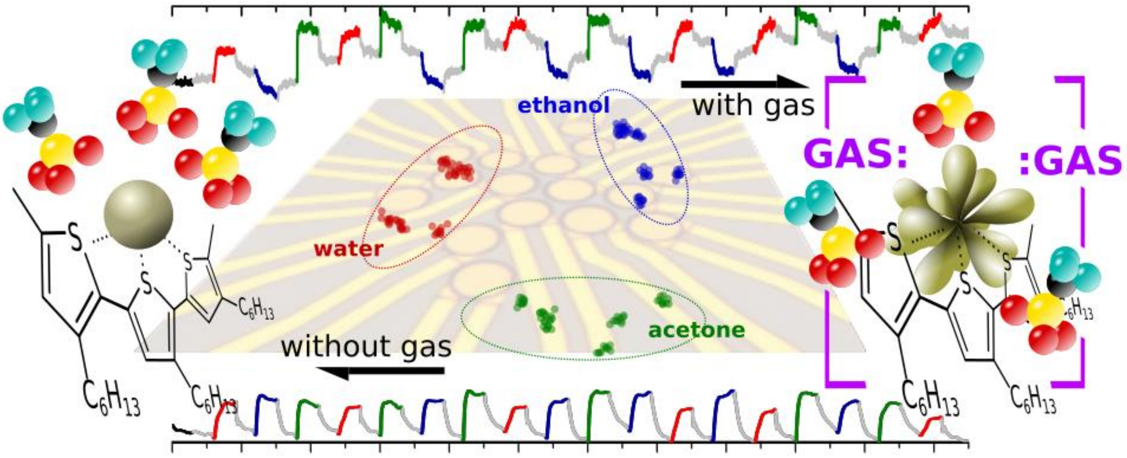
Abstract:

Conducting polymers can sense gases, however, it is mostly the dopant that dictates which ones: Here we show that a single conducting polymer discriminates gas-phase water, from ethanol, from acetone, on demand, by varying the nature of its dopant.[1] Seven triflate salts are evaluated as mild to strong p-dopants for poly(3-hexylthiophene) in sensing micro-arrays. Based on the nature of the salts, each material shows a dynamical pattern of polymer conductance modulation that is specific to the exposed solvent vapors. By multivariate data analysis, we show that the two mildest ones used in an array can be trained to reliably discriminate the three gases, proving that integrating one single conducting polymer suffices to build the input layer of a resistive nose. Moreover, the study points out the existence of tripartite donor-acceptor charge-transfer complexes responsible for chemo-specific molecular sensing. By showing that molecular acceptors have duality to either p-dope and coordinate volatile electron donors, such behavior can be used to unravel the role of frontier orbital overlapping in organic semiconductors and the formation of charge-transfer complexes in molecular semiconductors.



Graphical abstract displaying the molecular mechanistics proposed to justify the observed dynamical resistance modulation patterns (top Dy(OTf)$_3$-doped, bottom Fe(OTf)$_3$-doped) of P3HT exposed to water (red), acetone (green) or ethanol (blue) overtime, and for which Principal Component Analysis shows an optimal clustering for the three gases only by varying the nature of the dopant on P3HT (background : microscope picture of the micro-sensors used in the study).

[1] Boujnah A, Boubaker A, Kalboussi A, Lmimouni K & Pecqueur S, Mildly-Doped Polythiophene with Triflates for Molecular Recognition (submitted)

Poster

New liquid-crystalline semiconducting (PBTTT)-based polymer : from synthesis to organic field-effect transistor properties

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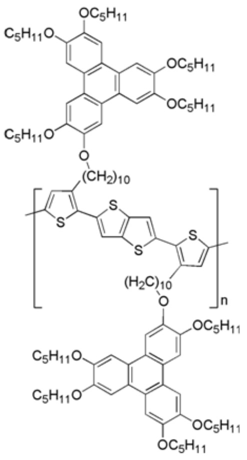
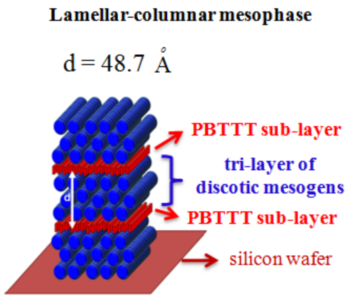
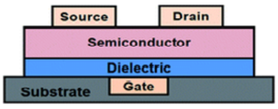
π–Conjugated macromolecules have attracted much attention due particularly to their semi-conducting properties which explain their integration into organic electronic devices, such as organic light-emitting diodes (OLEDs)[1], organic photovoltaic cells (OPVs)[2] and organic field-effect transistors (OFETs)[3]. In this field, one challenge is to improve the device performances, one way being to get higher charge carrier mobility. Such enhancement can be obtained in preparing ordered materials able to form highly organized thin film morphologies from solution processing[4].

On the one hand, Poly(2,5-bis(3-alkylthiophen-2-yl)thieno[3,2-b]thiophenes)(PBTTT) derivatives demonstrated high charge carrier mobilities and are efficient materials for OFET elaboration. On the other hand, triphenylene-based discotic mesogens can spontaneously self-organize to give columnar nanostructures by the stacking of their polyaromatic cores, providing an efficient pathway for a unidirectional charge carrier transport along the column[5]. In this context, herein we designed and prepared a new macromolecular architecture based on PBTTT polymer chain as backbone and triphenylene mesogens as side groups.





Model of self-organization



Output characteristics

$\mu\ h^+ = 1.2\text{x}10^{-5}\ cm^2/Vs$

The obtained polymer (PBTTT-Tri) was characterized by appropriate analytical techniques (1H NMR, 13C NMR and SEC) and its thermal behavior was studied by Polarized Optical Microscopy (POM) and Differential Scanning Calorimetry (DSC). The self-organization property of PBTTT-Tri was investigated by temperature dependent Small-angle X-ray Scattering (SAXS) and Grazing-Incidence Wide-Angle X-ray Scattering (GIWAXS). The results showed that the material presents a lamellar-columnar arrangement that can be oriented on surfaces. Moreover, the preliminary charge transport properties of PBTTT-Tri in thin films were examined in OFET configuration, and a p-type conduction with a hole mobility around 1.2 x 10-5 cm2 V-1 s-1 was observed.

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ELECMOL 2021
10th INTERNATIONAL CONFERENCE
ON MOLECULAR ELECTRONICS

CONFERENCE SCHEDULE

NOVEMBER 29 - DECEMBER 2 | 2021

DAY 1
NOV 29 | MON

10:00-13:00
Registration

13:00-13:30
Opening

Time	Chair	Speaker
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

Time	Chair	Speaker
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

Time	Chair	Speaker
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

Time	Chair	Speaker
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

Time	Chair	Speaker
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

Time	Chair	Speaker
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

Time	Chair	Speaker
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

Time	Chair	Speaker
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

Time	Chair	Speaker
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

Time	Chair	Speaker
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

Time	Chair	Speaker
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

Time	Chair	Speaker
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

Time	Chair	Speaker
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

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

17:20-18:00
Poster Prize & Closing

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HTDS
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