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Organic Nano-photonic

Nanophotonics: principles and applications

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Interaction of light with nanostructured materials gives rise to nanostructured optical waves, i.e., to electromagnetic fields varying strongly at the nanoscale, opening exciting possibilities for surpassing the classical diffraction limit and molding the flow of light at length scales far below the optical wavelength. Using carefully designed nanostructures light can be manipulated in fascinating new ways that are impossible to achieve with natural materials and in conventional geometries. This control over light at the nanoscale led to unveiling new physical phenomena and empowered many applications, including integrated optical circuitry, optical processing, super-resolution microscopy, quantum information technologies, bio- and medical sensing. In this talk, main principles and applications of nanophotonics are briefly overviewed with the emphasis on metallic nanostructures and surface plasmon-based (plasmonic) configurations for nanophotonics.

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Organic Nanophotonics

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Nanophotonics deals with the generation, modulation, guiding and detection of photons in a confined system at the nanoscale. Utilizing organic functional molecules as the building blocks of nanophotonic materials and components has great potential due to the multiple advantages, including the molecular design ability and tailorable properties. In this talk, the main focus is on organic crystalline nanowires, detailing the mechanism that led to their growth and exemplifies the linear as well as non-linear photonic properties. The development of destruction-free transfer enables fast and large-scale integration of highly oriented organic nanowires into semiconductor, metallic electronic or photonic platforms. Finally, future potential of organic nanowires is highlighted by presenting hybrid photonic/plasmonic platforms as passive and active nanoplasmonic elements.

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Beyond the 'pre-programmed' surface-confined supramolecular self-assembly - Towards nano-optics at surface

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A general strategy for simultaneously generating surface-based supramolecular architectures on flat sp²-hybridized carbon supports and independently exposing on demand off-plane functionality with controlled lateral order is highly desirable in view of the noncovalent functionalization of graphene.

With this aim, we recently developed the Janus tecton concept, a new Janus material [1 – 2]. This is a molecular three-dimensional (3D) building blocks consisting of two faces linked by a cyclophane-type pillar. One face is designed to steer 2D self-assembly onto C(sp²)-carbon-based flat surfaces, the other allowing for the desired functionality above the substrate with a well-controlled lateral order.

Here, we provide for the first time a versatile molecular platform [1] based on a library of new 3D functional nanostructures/Janus tectons able to form surface-confined supramolecular adlayers [1 – 3] in which it is possible to simultaneously (i) steer the 2D self-assembly on flat sp²-carbon based substrates [4] and (ii) tailor the external interface above the substrate by exposing a wide variety of small terminal chemical groups and functional moieties [1]. This approach is validated through the self-assembly study by scanning tunneling microscopy (STM) at the liquid-solid interface and molecular mechanics modelling.

The successful self-assembly on graphene, together with the possibilities to transfer the graphene monolayer onto various substrates and to transpose this approach to other 2D materials (h-BN), should considerably expand the domains of application of our functionalization strategy [1]. In this context, we recently demonstrated the first fluorescent supramolecular self-assembly on graphene with a specifically designed and synthesized three-dimensional (3D) Janus tecton.

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Experimental - Synthesis - Numerical simulation

X-ray Diffraction Using Grazing Incidence Techniques: Characterisation of Surfaces and Thin Films

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X-ray scattering techniques are widely used to characterise the structural properties of organic materials in terms of their crystalline and morphological features like type of phase, molecular packing, preferred orientation of molecules, crystallinity, etc. In case of organic thin films specific experimental techniques are required. The tutorial talk will introduce x-ray scattering techniques using grazing incidence conditions of the primary beam, namely x-ray reflectivity and grazing incidence x-ray scattering. The fundamental principle of these two methods will be discussed in terms of the optical properties of x-rays, a short comparison to analogous techniques using neutron beams will be drawn. The experimental possibilities of these methods will be introduced on basis of thin films of the molecule dioctyl-terthiophene. Special emphasis will be drawn on the interface properties of organic films in terms of surface and interface roughness and on the molecular order at surfaces.

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Transversal topic

Implement and evaluate the problem-solving approach

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”How much decreases the temperature of a glass of water when an ice cube melts in it?
” This question, asked with the thermodynamic data of water and without any guidance is one of the ” problem-solving ” given in tutorials to students who follow the module” Energy and entropy ” at UPMC (1st year - physics chemistry geoscience curses). The aim of this activity, intermediary between the guided exercise and the project is to conduct the student to mobilize knowledge, skills and competences to address a situation in which he must achieve a specific goal, but where the path to follow is not provided. How can this active pedagogy help to manage the diversity and heterogeneity of our students without increasing the number of specific modules and fragmenting the curriculum? How does it help the students to be more active in their training? How to prepare students to address an exercise in ”problem-solving”? How to evaluate the work done when various paths can lead to the result? These issues will be addressed through an experiment conducted for 5 years in the science curriculum and Po science and science and law (3 ECTS - 60 students) and then extended since 3 years this year in L1 module ”Energy and Entropy” portal PCGI (9 ECTS - 450 students, 18 groups).

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Molecular electronics

Single molecules interrogated in solid-state devices

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One of the challenging goals of molecular electronics is to understand and master single-molecule electronic devices. Based on recent progress employing three terminal solid-state devices it is possible to interrogate a single molecule in a metal gap by direct observation of vibrational, electronic and magnetic spectral details. The talk will focus on new insight into the physics and chemistry of such molecules in particular the influence of metal electrodes on the molecular energy spectrum, controlling molecular spin by external electrical fields, and progress towards chemical preparation of single molecule devices and molecular devices more broadly in which the molecule/metal interface can be controlled with sufficient precision.

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Self-Assembled Single-Molecule Electronic Systems

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Recent years have seen progress in several areas regarding single molecule electronic devices. A number of interesting structure–property relationships have been observed, including vibronic effects, spin transitions, and molecular electronic interference known as quantum interference. Together, these observations highlight what the rich opportunities in molecular design might bring in terms of advanced device properties.[1] Pertinent challenges in the field of are related to development of high yield preparative procedures for fabrication of single molecule devices in a parallel and reproducible way. With these two lectures we introduce methods for realisation of single molecule electronic devices and discuss how the field can move forward in terms of developing methods for parallel fabrication of multiple single molecule electronics devices. We discuss methods for the formation of the nanogaps as well as methods attempting to achieve single molecule functionality in each individual device.[2] Examples include fabrication of single molecule devices by in-situ growth of gold nanorods,[3] formation of nanogaps via deterministic self assembly of gold nanorods,[4] In the second lecture we will discuss various means of integrating advanced molecular function such as molecular switches into single molecule electronic devices.

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Electrochemical approaches for molecular electronics

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The talk will include two different parts representing some of our activities in the domain of molecular nanoobjects. First, electronic communication inside molecular systems is very complex since nuclear motions affect electronic levels and thus the final efficiency of the device. In this field electrochemistry has proven to be relevant to estimate the rate of electron transfer from a redox center towards an electrode. For practical applications, there is a need for a fast signal transduction. However, this raises the difficulty of finding a method with an adapted temporal resolution. We rely on ultrafast voltammetry for this purpose, and several examples of kinetic rates determination will be depicted. A first category will be molecular wires adsorbed onto electrodes. Here, a single electron is transferred per molecule. Larger systems such as dendrimers bear a multiplicity of redox centers, some of them being too far from the electrode to allow a direct communication. However a redox reaction can still occur by successive electron hopping between neighboring entities. On these large systems, we could access to the intramolecular dynamics of the redox entities.

On the other hand, complementary information can be obtained by performing conductance measurements relying on the the Scanning Tunneling Microscopy Break Junction method. Here a steady state value (the resistance of the molecule) is obtained, but at the single molecule level. It was observed that kinetically fast systems indeed display larger conductances. Electronic coupling factors for both experimental approaches were therefore evaluated based on superexchange mechanism theory. This suggests that coupling is surprisingly on the same order of magnitude or even larger in conductance measurements whereas electron transfer occurs on larger distances than in transient electrochemistry. It is thus very different to have a steady state flux of electrons through a single molecule than to localize a single electron per redox center in a large collection of molecules. Furthermore, in electrochemical conditions, the conductance changes with the electrode potential (at constant bias), mimicking a single molecule field effect transistor for which the gate electrode is the reference electrode.

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Electronic properties of organic layers on oxide-free silicon for the next generation transistors

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Organic molecules can be viewed as promising building blocks for electronics. For example, the new AMOLED displays (Active-Matrix Organic Light Emitting Devices) are now currently used in cell phones and have just become cheaper than the conventional LCD (Liquid Crystal Displays). However the control of the electronic processes occurring in molecular architectures requires a high control of the morphological organization since one crucial aspect is the connection between molecules and electrodes. This talk will address the case of molecules connected to silicon interfaces and clarify charge transport is understood. Using scanning tunnel microscope (STM) and conductive AFM (c-AFM), we show how to use these properties for designing organic transistors, such as a single electron transistor.

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Transversal topic

The European job market for doctorates: an overview

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Around one-fifth of the doctoral candidates of the European Union are working in universities outside of their home country. Whereas figures of researchers under fixed term contracts show similar results, permanent positions in international mobility are substantially less frequent. Nevertheless, Europe is, as we all know, far from being homogenous. As a consequence, those international mobility figures are extremely different from one country to another. While some European countries have a surprising amount of native researchers, others mostly rely on foreign scientists. This brings interesting international mobility opportunities.

Although early stage researchers are still inadequately informed about it, the job market for doctorates is, however, not limited to academia since nearly half of the EU researchers are working in the private sector. Furthermore, many employers see the doctorate as a high-level qualification bringing many advanced transferable skills, in a great panel of professional sectors, not necessarily in research-related areas. That creates a strong overall demand, which is ready to meet the observed increased supply. The specificities of the different situations and opportunities are, again, highly dependent on the sector as well as the country.

The point of this presentation is to give the audience an overview of the job market for doctorates in Europe. Though the situation is extremely complex and country-specific, we will bring forward interesting trends in academic and non-academic research as well as in non-research-related areas.

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Nano bio - medecine

Nanotechnology to nanomedicine: are we about to cross the blood brain barrier?

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The brain is always confronted with the dilemma of the protection from noxious substances from the blood and the delivery of vital metabolites. Endothelial cells, forming together with other cells the blood-brain barrier (BBB), are known as the "gatekeepers" of this trafficking. On the one hand, the protection from toxic molecules is achieved by the obstruction of the paracellular pathway with tight junctions, that fuse brain capillary endothelia into a continuous tubular cell layer. On the other hand, vital molecules are transported from the blood by means of active trans-cellular mechanisms. Many interests are focused on the BBB, with the aim to exploit these mechanisms for successful delivery of drugs across the barrier. About 98 per cent of today's medications cannot cross the blood-brain barrier in significant quantities. Drugs such as most antipsychotics, sleeping aids and antidepressants are smaller than 500 daltons and can sneak through. But they're in the two per cent of drugs that can get through. Some small, lipid-soluble drugs do cross the BBB simply by diffusion through the cell membrane, and others enter successfully via specialized transporter proteins. Many larger molecules, such as antibodies and enzymes, however, can't get through. Recently, the emerging field of nanotechnology has generated new promises to solve this problem. Which method is most successful will likely depend on what type of molecule you are going to target to the brain.

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Basic Concepts in Cell-Materials Crosstalk at Nanoscale

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In the last 15 years nanotechnologies have been largely applied to develop novel functional biomaterials. The key-challenge is to succeed in building functional biomaterials-cell interfaces able to control cell activities and direct their fate, i.e., in short, able to globally manage the cell-material crosstalk. In this framework, the basic objective consists in identifying which nanoscale surface factors are intrinsically relevant to the cellular processes, providing the elements of the cell-material communication code. This Lecture is therefore aimed to set the basic landscape, by focusing the attention on the material surface properties at nanoscale which have been reported to affect the strength and the nature of the cell-material interactions (participating in the same material-cytoskeleton crosstalk pathway via adhesion plaque), including topography, confined biological cues, mechanical and electrical properties. Among the many possible forms of surfaces nanostructuring, the Lecture will further suggest a few examples of self-structuring, patterning and nano-confinement as well as strategies to obtain the biomolecule "orientation", as propaedeutic steps to construct multifunctional bioactive platforms, integrating different possible biological actions. Finally, the concepts of "cell instructive" and "programmable" surfaces will be shortly discussed. Keywords: cell-material interaction; biomaterials; biomolecular signals; topography; cell adhesion; patterned substrates

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Bio-nano hybrid surfaces

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Nanostructuring and, in some cases, adsorption of biomolecules are often the starting points to make functional surfaces for, as examples, i) material integration in the human body or ii) biofilm construction on any type of material in a natural environment ; some biomolecules, in particular peptides, are indeed frequently utilized to control the reactivity or passivation of solid materials. It is thus crucial both to understand the interaction of biomolecules with solid surfaces and, deduce ways of immobilizing them, in a controlled geometry. Mostly based on a surface science approach, sometimes enriched by calculations, this presentation will focus on basic investigations of the adsorption short peptides on metal, nanostructured, surfaces. We will see how the mode of adsorption and geometry of a peptide may direct the growth of single or multilayers, and how adsorption of peptide enantiomers can imprint chirality and induce enantioselective recognition, or yield anti-adhesive surfaces.

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Magnetic silica core shell nanoparticles for biomedical applications

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Magnetic nanoparticles are widely studied since several decades for biomedical applications. They are still used in clinic as negative contrast agent (T2) in Magnetic Resonance Imaging. Using them as drug carriers could allow guided delivery thanks to magnetic targeting and combined therapy while using magnetic hyperthermia to kill cancerous cells. In diagnostic, they can be used as a diffusing solid phase, confinable while applying a magnetic field gradient. Core shell magnetic nanoparticles are made of few magnetic nanoparticles coated by a non-porous silica shell. The silica shell can be easily doped with fluorescent molecules, useful for the detection in a diagnostic chip or cell imaging. The silica shell surface is a versatile platform for functionalization, with drugs, protein, DNA... depending on the aimed application. In this talk, I will present some results about the synthesis of twice functionalized silica core shell nanoparticles and their use in different context, for diagnostic or therapy.

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Experimental - Synthesis - Numerical simulation

Modeling devices for photovoltaics : insights from ab-initio approaches

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A general overview of ab-initio approaches essentially rooted on Density Functional Theory, for the description of the structural and electronic properties ruling the macroscopic behavior of devices for photovoltaics applications, will be given through selected examples. In particular, this talk will be focused on the computational approaches enabling the description and the design of dye sensitized solar cells (DSSCs) and quantum dot sensitized solar cells (QDSCs) in order to highlight both their success and their current limitations. Examples of the application of these methods -ranging from the modeling of photovoltaic characteristic of DSSCs to the relation between the morphological and the charge transport properties in hole transporter materials for energy devices- will be provided.

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Original Polymer Synthesis through an Organometallic Approach

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The first polymerization exploiting the carbenic reactivity of homogeneous gold catalysis has been devised. In the presence of a gold catalyst, monomers incorporating both a propargylic ester and an alkene moiety polymerized through a metallocarbene generation/cyclopropanation sequence to afford the corresponding macromolecules. This approach constitutes an unprecedented example of cyclopropanation-based polymerization and allows access to original macromolecule skeletons. The latter were then analyzed from the viewpoint of conductivity and showed some promising properties.

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Chemical Synthesis of inorganic nanomagnets

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Metallic nanoparticles and nanohybrids will initiate important development in nanotechnologies due to their specific chemical and physical properties (*i.e.* in catalysis, magnetism, optics, etc) and new development in sustainable energy (*i.e.* fuel cells). It is now well known that these properties are mainly controlled by the fine tuning of structural parameters such as the size, shape, crystallinity and composition. In order to study these specific properties, a wide variety of both chemical and physical routes have been developed for the synthesis. In particular, one of the specific challenges in the synthesis is to control and to characterize the nanohybrids at the nanometer scale. Concerning their fabrication, the chemical bottom up approach, is ideal to design this specific class of nanomaterials due to its versatility, facility and low cost. In the following, we review some of the most classical chemical routes to produce such nanohybrids focusing on the case on cobalt and Co-Pt nanomagnets. We discuss the concepts of nucleation and growth for such objects and their consequence on their structural properties (size, shape, composition, ordering...).

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**Organic and Nano magnetism in
collaboration with 4th International
Workshop on Novel Magnetic and
Multifunctional Materials**

Molecular magnetic systems grafted on a surface

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In this course, I shall focus on the original properties that are exhibited by molecular magnetic systems when they are grafted on a surface.

I shall first present the Single Molecule Magnets (SMM) with their unique property associated to the quantum relaxation of magnetization. Then I shall review how such unusual properties are modified when SMMs are deposited on either a metallic, an insulating or a ferromagnetic surfaces. Emphasis shall be brought to the nature of the magnetic ions with a special attention to the orbit and spin contributions to the magnetization. The main technique of investigation is x-ray magnetic circular dichroism and for which the basic concepts shall be rapidly introduced. In a second step, I shall present various thermomagnetic and photomagnetic systems where the magnetic properties can be triggered by an external stimulus such as temperature or light. The case of Spin Cross Overs (SCOs) shall be reviewed with a special attention to cooperativity when SCOs are deposited on a surface. I shall also present systems where a charge transfer is at the origin of the photomagnetism. Again the finite size of the charge transfer units and the observed modifications when the systems are deposited on a surface shall be addressed.

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Recent progress in hybrid organic/inorganic heterostructures for potential magnetoresistive applications

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My course will be focused on the recent progress in the study of a new class of devices based on hybrid inorganic metal and organic semiconductor heterostructures and their potential for magnetoresistive applications.

Organic spintronics, a fusion between organic electronics and spintronics, is a new and promising research field where organic materials are used to mediate or control a spin-polarized signal. The field of organic spintronics is particularly attractive due to the potentially very long spin relaxation times in OSC. One of the main advantages with OSC is that they allow chemical tuning of their physical properties such as electronic gap, injection barrier, mobility, spin-orbit coupling and hyperfine interaction.

Basically, organic spintronics can be divided into two classes: OMAR (organic magnetoresistance) and OGMR (organic giant magnetoresistance). OMAR devices structures are based on one OSC layer sandwiched between non-magnetic electrodes. OMAR effects, - the change in resistance with magnetic field, - result from intrinsic magnetic field effects on the electronic levels involved in charge transport. The latter - organic spin valves (OSV or OGMR) are different from OMAR since they contain ferromagnetic electrodes. They are constituted of three active layers: a first, "soft" ferromagnetic electrode layer; a spacing layer (OSC); and a second, "hard" ferromagnetic electrode layer. They are designed to exhibit either a high or low resistance, depending on the carrier electron spin alignment in the magnetic layers.

I will present an overview of such effects and the associated materials, techniques and models used in their study.

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Enhancing the magnetic anisotropy of maghemite nanoparticles via the surface coordination of molecular complexes

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Superparamagnetic nanoparticles are promising objects for data storage or medical applications. In the smallest-and more attractive-systems, the properties are governed by the magnetic anisotropy. Here we report a molecule-based synthetic strategy to enhance this anisotropy in sub-10-nm nanoparticles. It consists of the fabrication of composite materials where anisotropic molecular complexes are coordinated to the surface of the nanoparticles. Reacting 5nm g-Fe₂O₃ nanoparticles with the [CoII(TPMA)Cl₂] complex (TPMA: tris(2- pyridylmethyl)amine) leads to the desired composite materials and the characterization of the functionalized nanoparticles evidences the successful coordination-without nanoparticle aggregation and without complex dissociation-of the molecular complexes to the nano- particles surface. Magnetic measurements indicate the significant enhancement of the ani- sotropy in the final objects. Indeed, the functionalized nanoparticles show a threefold increase of the blocking temperature and a coercive field increased by one order of magnitude.

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A chemist's tool box for integrating magnetic molecular architectures on surfaces

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One of the strengths of inorganic molecular Chemistry is its ability to produce a variety of molecular architectures whose amplitude is only limited by the imagination of the synthetic chemist. On the other hand, by essence, each synthesis produces molecules that are all perfectly identical in terms of structure and size. These two assets allowed molecular magnetism, a discipline at the edge between Chemistry and Physics, to study and elucidate mechanisms leading to magnetism in molecules. It also allowed the discovery of new and specific phenomena such as the blocking of the magnetization and the quantum tunnelling of the magnetization on single molecules. Today, inorganic chemists have to face another challenge: the integration of molecules bearing properties of interest into functional devices. This presentation aims at giving a few examples of hybrid materials allowing the study of magnetic properties of confined molecular architectures and the perspectives it opens towards molecular spintronics.

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Experimental - Synthesis - Numerical simulation

Scanning Probe microscopies for Soft matter and nanoparticles

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In this talk I will provide an overview of Scanning Probe Microscopies when they are devoted to the study of organic materials, spanning from organic monolayers, where mainly Scanning Tunneling Microscopies (STM) are used, organic films where mainly Atomic Force Microscopies (AFM) are used to biological materials where a new mode of AFM can be used, the so-called "peak force mode". I will show in particular that AFM constitutes a useful tool for topography characterization, underlining as well a number of possible artifacts, but also that spectroscopies can be associated with the various modes of Scanning Probe Microscopies. I will indeed show that the density of state of a material can be locally probed, but also the Hamaker constant and even the Young modulus or the hydrophobic/hydrophilic character of an interface.

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Transversal topic

Communicate on your scientific results

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When a scientist has some good results, proved by an article accepted in a science journal, his job isn't finished. He or she has to communicate beyond the scientific community. Why ? There are many reasons for that : improving his scientific reputation, searching funds, informing the citizen, initializing industrial collaborations... Communication skills are today one of the essential skills for a scientist.

Unfortunately, scientists rarely know how to do that. But they can be helped by the communication services of their employer, which can for example make a press release about the result, and send it to journalists. They can also learn how to vulgarize and communicate for different kinds of public.

This talk aims to give a few keys to communicate efficiently.

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Organic devices

Scope and challenges for organic solar cells in the current race to performance

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After a brief state of art of the challenges of renewable energy and more sepcifically of the solar cells, the place of organic solar devices will be discuss in front of competitive technology such as Perovskite or CIGS. Indeed organic solar cells reveal numerous advantages competing with higher efficiency devices. Despite that, numerous challenges are emerging with the constant increase of the performance of organic solar cells (OSC); the optimization at each steps of the electronic processes becomes critical. We will pay a specific attention to the charges collection at the electrode and more specifically at the anodic side of the device emphasis the energetic leveling of each material involve.

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OLED for display and lighting applications: current issues and future directions

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Organic Electronics have received a lot of attention during the last years and advancements are leading to commercial products. Organic Light-Emitting Diodes (OLEDs) have already entered the mass production market in small size displays (smart phones, ...) or larger area display devices for OLEDtelevisions. However, the request in the market continues to grow for low-power, low-cost and flexible devices. OLEDs have also shown a great potential for lighting applications and worldwide research is ongoing to create high-brightness, high efficiency and long life white OLEDs for lighting. This presentation will give an introduction to OLED operation mechanisms and review recent insights into OLEDs materials, device structures and manufacturing processes. Some recent results from our group on the use of new host materials and TADF emitters will be presented.

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Organic transistors

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Organic transistors are sometimes claimed as an alternative to conventional microelectronics. However, despite tremendous progress since their first appearance, they have not known any commercial application to date. In this lecture, we will delineate what differentiates organic transistors from their inorganic counterparts. We will next focus on their most promising applications, in particular in the field of biomedical devices.

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Poster

A facile synthesis of a thiophene-based molecule as hole transporting material in mixed cation-based perovskite solar cells

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Recently the progress in the application of hybrid organic-inorganic perovskite as a light-absorber in solar cells has raised the power conversion efficiency from 3.8% to over 22% in few years, making these cells as spearhead in thin film PV technology. This unprecedented increase in PCE of perovskites based solar cells motivated researchers to optimize the materials, the architectures and layers configurations, in order to improve further the photovoltaic properties. In all these architectures Spiro-OMeTAD remains the best material used in Hole Transporting Layer as electron blocking and p-type material. However, Spiro-OMeTAD is too expensive due to its multistep synthetic route and complex purification, which raises its commercial price. Moreover, it doesn't performs good in its pristine form, so it needs a p-type additives in order to enhance hole mobility and conductivity. Recently researchers are focusing in the design of novel small organic molecules as cheaper and efficient Hole Transporting Materials (HTMs). Here we present an easy-to-be-synthesized thiophene-based molecule that has been used as HTM in mixed cation perovskite-based solar cell and that shows encouraging results in order to achieve efficient and commercial accessible devices.

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Adsorption of aromatic molecules on the platinum (111) surface

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Aromatic molecules are promising building blocks for active and carrier-injection layers in organic electronics. The interaction of the first adsorbed layer of such molecules is fundamental in determining the growth of a film on a substrate. For this reason such adsorbed systems have to be carefully modelled. The van der Waals (vdW) interaction plays a crucial role in determining the correct adsorption geometry and energy [1]. Platinum can be used in devices as a high work function electrode. Our study investigates two members of acene family, namely benzene (Bz) ($C_6 H_6$) and pentacene (Pc) ($C_{22} H_{14}$), adsorbed on the (111) surface of Platinum (Pt). We determine for both systems the adsorption energetics and configuration for different geometries by the means of density functional theory, also accounting for vdW dispersion. The simulations have been performed using Quantum ESPRESSO (QE), VASP and FHI-AIMS employing Grimme D2 [2], screening-corrected Tkatchenko-Scheffler [3, 4] (TS surf) and optB88-DF [5] vdW correction schemes. For both Bz as well as Pc, independent of the vdW correction employed, a strong hybridization of the molecule with the substrate is observed. The most stable configuration of the Pc on Pt (111), with the central carbon ring at bridge position, displays a slightly bent profile which is in good agreement with experimental Scanning Tunnelling Microscopy (STM) images.

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Architecture contributions and attenuation of short channel effects in organic transistors

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Organic thin film transistors still suffer from an insufficient stability and cannot compete with the performance of their inorganic counterparts. Nevertheless, highly promising advances in switching speeds were achieved upon aggressive scaling of device dimensions such as the channel length and the gate dielectric thickness [1]. The benefits of reducing the channel length, i.e., the separation of source and drain are, however, counteracted by non-desired short channel effects and increasingly dominant contact resistances. Introducing local doping near the metal electrode – semiconductor interface has been demonstrated to efficiently suppress the latter.[1] Theoretical work indicates that, without the benefit of doping, the contact resistance is strongly related to the efficiency of injection at the metal-semiconductor interfaces and depends not only on the carrier mobilities and injection barriers, but also on the device dimensions, the orientation of the injecting surface with respect to the semiconductor-insulator interface, and the point of operation. [2]

To provide a solid basis for a deeper understanding of the doping-induced effects at the contact interface, we investigate the interplay between short channel effects and injection for undoped devices. We utilize two-dimensional drift-diffusion-based simulations including the self-consistent consideration of thermionic and tunneling injection, interface recombination, and back drift, to determine the contact resistance and short channel effects directly from the simulation of the device at a given point of operation. The considered channel lengths vary by three orders of magnitudes, i.e., range between several micrometers to 300 nanometers and below. We particularly focus on how the onset and the extent of short channel effects for given material properties depend on the injection barrier and the actual device architecture, i.e., the staggered (top-contact bottom gate) or the coplanar (bottom-contact bottom-gate) device configuration.

Accepting bulk current as the source of saturation loss, we achieve a modest suppression by introducing a mesa/dielectric body in the active region to reduce the channel width and eliminate bulk current [3]. Further variations of this mesa structure are presented, pointing at which ones are desired to get closer to the ideal Gradual Channel Approximation behavior.

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Composite Porous Silicon-Crystalline Silicon microcantilevers for biological recognition

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Biosensing technology is a rapidly advancing field that benefits from the possibility to use the properties of functional advanced materials to analyse biological systems. In particular, nanomechanical systems are very attractive for biological sensing since mechanical interactions are fundamental to biology. Indeed, nanomechanical devices allow measuring forces, displacements and mass changes from cellular processes, and provide high sensitivity and fast responses, which is necessary for the observation of biological processes [1]. On the other hand, among all the functional materials, PSi constitutes an ideal substrate for developing new chemistries owing to its biocompatibility, well-established fabrication methods and large adsorption surface area, which allows an enhanced sensitivity [2]. In this work, we will start by reviewing the processes for the PSi formation on microcantilevers and their biofunctionalization in order to trigger its sensitivity as biosensing platform. Secondly, we will describe current approaches based upon modification by self-assembled silane monolayers, which critically depend on the type of process for the activation of PSi. Depending on the molecular structure of the monolayers, the surface presents hydrophobic/hydrophilic properties, allows a molecular selectivity, and a local control of the biomolecular interactions. Dynamic experiments involving condensation and evaporation of water on the functionalized PSi samples will be carried out by wetSTEM in order to study and characterize their interaction with water. The surface of the functionalized material will then be biologically activated for the detection of specific genomic or proteomic species applying surface immobilization techniques. Finally, the process of formation of the biorecognition interface will be applied to composite porous silicon-crystalline silicon cantilevers and preliminary sensing results will be shown.

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Concentrated dispersions and melts from micellar solution: computer simulation by dissipative particle dynamics

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It is well-known that the process of microphase segregation, that occurs in the melts of thermodynamically incompatible block-copolymers, leads to the formation of ordered structures with different morphologies (spherical and cylindrical domains of one phase into another, lamellar structures, gyroid structures, etc). However, the formation of a segregated film with well-defined order is a complicated problem from the viewpoint of technical implementation owing to a number of labor-intensive procedures, such as selection of common solvent, regime of solvent evaporation and film annealing. To investigate the production of nano- and micro-structured films, the approach, which is based on film formation by solvent evaporation may be proposed. In this research we study the films formed by block-copolymer micelles (core-shell particles) by means of DPD (dissipative particle dynamics) simulation technique. We test the melt stability and compare melt structure with previously obtained results for preliminary formed macromolecular objects.

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Excitation of surface plasmon polaritons in nanostructured organic hybrid systems

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Organic plasmonic hybrid systems are promising components for next-generation nanophotonic devices, because they can serve as active plasmonic elements in nanophotonic circuits, converting optical signals into plasmonic signals and vice versa [1]. Moreover, exchanging noble metals with recently recognized plasmonic materials (e.g. TiN), gives the opportunity to design and fabricate low cost and CMOS compatible systems, which can be utilized for plasmon generation, modulation and sensing [2].

In this work, we focus on both linear and non-linear optical properties of organic nanofibers (ONFs), namely photoluminescence and second harmonic generation, which subsequently excite surface plasmon polartion (SPP) [3][4]. Organic material transferred from the growth to a nanostructured surface, creates a system, which allows us to explore exciton-plasmon coupling. To explore the fundamental properties of the hybrid system, we perform time-resolved photoluminescence spectroscopy, conventional reflection spectroscopy and fluorescence lifetime imaging microscopy. Furthermore we compare our experimental to numerically obtained results from finite-difference time-domain calculations. The presented studies contribute to a better understanding and control of hybrid-mode systems, which are crucial elements in future designs of low-loss photonic energy transfer devices.

Keywords: surface plasmon polaritons, organic fibers, hybrid modes, exciton-plasmon coupling, reflection spectroscopy, fluorescence lifetime imaging microscopy,

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Femtomagnetism in graphene induced by core level excitation of organic adsorbates and the role of electron transfer

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We predict the induction or suppression of magnetism in the valence shell of physisorbed and chemisorbed organic molecules on graphene occurring on the femtosecond time scale as a result of core level excitations and electron transfer at the interface [1]. For physisorbed molecules, where the interaction with graphene is dominated by van der Waals forces and the system is non-magnetic in the ground state, numerical simulations based on density functional theory show that the valence electrons relax towards a spin polarized configuration upon excitation of a core-level electron with the LUMO shifting closer to the Fermi level to accommodate the additional charge and screen the positive core hole. The system is magnetic until the core electron de-excites via one of the several electronic decay channels [2,3]. The magnetism depends on efficient electron transfer from graphene and the corehole lifetime is in the femtosecond (fs) time scale. On the other hand, when graphene is covalently functionalized, the system is magnetic in the ground state showing two spin dependent mid gap states localized around the adsorption site [4].

The influence of a substrate is then considered for charge transfer between molecules and supported graphene. We focus on the resonant charge transfer lifetime of N-1s core excited 1,1'-Bipyridine adsorbed on epitaxial graphene/ Ni(111). In the ground state, even though the system is magnetic, there is no magnetic moment on the molecule. Upon photoexcitation, our calculations predict that charge transfer may occur bidirectionally to/ from the LUMO on a few-fs timescale in good agreement with experimental results [2] and differently from unsupported graphene where no itinerant states are available at the Fermi level.

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How does structure affect interfacial charge transfer? – isonicotinic acid on rutile(110)

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Charge transfer processes at interfaces in photovoltaic systems are strongly affected by temperature. In this context we analyze the effects of heat-induced structural fluctuations from a modeling perspective. In our approach we extract lifetimes of localized states on dye molecules attached to semiconductor substrates. The atomic motions of the adsorbate and substrate are sampled by taking snapshots from *ab-initio* density-functional-theory molecular-dynamics trajectories [1]. We effectively extend the slabs utilized in our dynamical calculations to full semi-infinite substrates with the use of a Green’s function approach [2,3]. At this level of theory we obtain time-averaged values of the charge injection times using several snapshots of the Car-Parinello simulations. We compare our results with core-hole-clock experiments of the same system finding a good agreement [4]. To include the perturbation inferred by the measurement technique we consider core-excited molecules in our simulations. This results in a lowered dependency on structural fluctuations of the energetic positions of the molecular level as compared to the non-excited molecule. This study enables the search for direct connections between structural parameters, resonance energies, and elastic charge transfer times scrutinizing the configurational space covered by the molecular dynamics simulations.

This project has received funding from the European Union’s Seventh Framework Programme under grant agreement no. 607323 [THINFACE]

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Influence of the protective DLC layer on organic plasmonic hybrid systems

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Organic plasmonic hybrid systems, consisting of a nanostructured metal substrate and organic nanofibers, have gained an increasing amount of attention due to their ability to generate, control and sense surface plasmon polaritons [1]. The most commonly used material for substrates in hybrid systems is gold, which is soft and therefore prone to mechanical deformations. It has been shown that the mechanical properties of the gold plasmonic substrates can be improved by applying a protective diamond-like-carbon (DLC) coating [2]. Nevertheless, the influence of the DLC layer on plasmonic hybrid systems has not been yet investigated.

In this work, we investigate plasmonic hybrid systems, consisting of 1-Cyano-quaterphenylene (CNHP4) nanofibers on top of gold nano-square arrays, covered with DLC layers of various thicknesses (25, 55, 105 nm). To confirm the field enhancement on top of the DLC layers, we compare the second harmonic response of organic nanofibers, located on plasmonic arrays, to those located on a plain gold film. Subsequently, we perform time-resolved photoluminescence measurements to verify a reverse interaction, where plasmonic coupling is considered as one of the loss channels for photoluminescence from organic nanofibers.

Our measurements reveal an optimum DLC coating thickness of 25 nm, for which the plasmonic substrate remains active. For thicker coatings (above 55 nm) we do not observe an interaction between the plasmonic substrate and the organic nanofiber. Our research explains the influence of the protective DLC layer on plasmonic hybrid systems, pointing out limitations in the coating thicknesses, which is a step-forward towards producing robust plasmonic substrates.

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Interface Engineering in Organic Semiconducting Materials for Solar Cells

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This work presents the synthesis of various organic polymers and copolymers with the intention to study the effect of chiral substituents on the packing and morphology of such materials in the solid state for their potential use in bulk heterojunction solar cells.

Conjugated alternating copolymer designed solar cells have the advantageous characteristics of highly tuneable optical band gaps. Additionally, selection of different polymer units and side chains can allow fine-tuning of the active layer morphology possibly resulting in increased efficiency. [1a][1b] Polymer based solar cells are produced by physical mixing of the 2 components and their efficiencies not only rely on the ability of the components to create interpenetrating domains throughout the active layer but many other factors such as the size of the optical band gap, absorption coefficient, charge carrier mobility, crystallinity, solubility and surface morphology.

Various units are under investigation with the core unit being diketopyrrolopyrrole (DPP), as its photochemical and thermal stability are now seen as vital properties for making stable and efficient solar cells. The core unit contains a planar bicyclic structure, which increases the possibility of strong π - π stacking interactions, [2] and polar carbonyl functionalities able to induce intermolecular hydrogen bonding. These factors can lead to close packing of the molecules in the solid state and well defined domains. The DPP unit is attractive as it presents a multitude of opportunities to modify and enhance the core structure. Thiophene DPP based polymers have been reported to feature high charge carrier mobilities and these species are electron donors so there is potential to control the size of the optical band gap by copolymerisation with electron withdrawing moieties. [3] Furthermore, the lactam N atom provides a site for addition of alkyl groups therefore allowing variation of the solubility of a resulting polymer or when left unalkylated, a site for hydrogen bonding interactions. [4]

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Investigation of Optical Properties of Diamond Like Carbon Thin Films with Embedded Silver Nanoparticles Employing Spectroscopic Ellipsometry

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Nowadays there is an increased interest in localized surface plasmon resonance (LSPR) of metal nanoparticles. At first and most commonly, LSPR of gold nanoparticles were investigated, because of its high response and stability [1]. However, gold possesses high absorption, which causes lower sensors sensitivity [2]. Thus new materials started to be investigated: silver [3], palladium [4], copper, platinum, nickel, tin, yttrium, aluminium [1]. Sensor applications is not the only field, where nanocomposites of metal nanoparticles in a matrix can be utilized. Potential fields of application are solar cell efficiency enhancement, perfect absorbers, photochemical reactions, antibacterial films and others [3, 5, 6].

Spectroscopic ellipsometry is an optical non-destructive measurement technique. It is commonly used to determine refractive index n and thickness of thin films d , but it can also provide results about extinction coefficient k , volume concentrations of materials in a composite and many more [7]. The main drawback of this technique is that it requires building an optical model, which subsequently requires some initial knowledge about the film. Mixtures of two or more materials (e.g. composites) have to be described using Effective Medium Approximation (EMA). Known materials are described by dispersion values from database, while unknown – by assigning dispersion laws with certain varied parameters. The actual properties of the film are derived through fitting simulated Ψ and Δ functions to experimentally measured. The goodness of fit is described by coefficient of determination R^2 and root mean square error RMSE [8].

In this work, the investigation of nanocomposite thin films, consisting of diamond like carbon matrix with embedded silver nanoparticles (DLC:Ag), is presented. Thin films with different silver content were deposited employing magnetron sputtering on two different substrates: fused silica and silicon. DLC:Ag on fused silica were used for investigation of absorption spectra. The spectra were obtained employing AvaSpec-2048 (Avantes) UV-VIS-NIR spectrometer. DLC:Ag on silicon were used for investigation with scanning electron microscope (SEM, FEI Quanta 200 FEG) and energy dispersive X-ray analysis (EDS, Bruker). Optical properties of all samples were

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investigated employing variable angle rotating compensator spectroscopic ellipsometer GES5-E (Semilab). 7 different angles of light incidence were used: 45 deg. – 75 deg. (step 5 deg.). The dispersion graphs of ellipsometric parameters Ψ and Δ were registered at wavelength range of 190-900 nm. Theoretical model was created and fitted to experimental data using Spectroscopic Ellipsometry Analyzer (SEA, Semilab) software.

Before fitting, experimental data was smoothed using build-in SEA function. 2-layer optical model was created to explain the thin film. Bruggeman EMA was chosen for DLC:Ag mixture. DLC was described by Cody-Lorentz dispersion law and silver was described by n & k values from database. Simulated Annealing fitting algorithm was chosen. Fitting results were in good agreement with experimental data: coefficient of determination reached 0.98 and root mean square error was up to 1.66. It was found out that the thickness of sample with 14.1 at% silver is 43.5 nm and is similar to what was expected. Its silver volume concentration is 22 % and refractive index at 632.8 nm is 1.56. The dispersion graphs for the thin film were also derived. The average size of nanoparticles is 3.5-5.1 nm.

Keywords: spectroscopic ellipsometry, sensor applications, nanocomposites, diamond like carbon, silver nanoparticles.

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Molecular Magnets: From the single molecule to the 3D self-assembly

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Real materials are not pure. Impurities can bring to light beautiful physics: they are crucial, for instance, in achieving the functionality of doped semiconductors. Indeed, sensitivity of a physical system to disorder can lead to elucidating details of electronic correlations and producing electronic states that are impossible in clean systems.

In particular, magnetic impurities in superconductors are able to reduce the superconducting BCS gap and may ultimately destroy the superconducting state. A single classical spin of a magnetic atom is able to create a localized bound state within the BCS gap (Shiba state). Consequently, a finite concentration of magnetic impurities can form an impurity band within the superconducting gap. The spatial decay of these bound states critically depends on the dimensionality of the system, i.e. it is increased by reducing the dimensionality [1].

The Pb/Si(111) system is one of the most remarkable examples of a 2D superconductor in which superconductivity arises in a single atomic plane of Pb [2, 3]. I will present preliminary results of the in-situ preparation (UHV conditions) of this system at room temperature and I will show its complex phases diagram. I will also illustrate the possibility to use Differential Reflectance Spectroscopy (DRS) in order to optically follow in real-time the temporal evolution of the thickness of Pb during its growth on the Si substrate.

The use of magnetic phthalocyanines as magnetic impurities by evaporating them on the Pb monolayer might lead to some advantages. For instance, playing with both self-assembly properties of these molecules and substrate anisotropy allows to tailor robust arrays of magnetic centers in 1D and 2D [4]. For this reason, is very intriguing to investigate the superconducting substrate-mediated interaction [5] between two Shiba States which could be used as building blocks for coupling coherently distant magnetic molecules. Such long-range coupling of magnetic impurities through a 2D superconductor could be an efficient way to create new topological phases exhibiting Majorana edge states.

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Multi-junction solar cells from DBP/C70 reaching open-circuit voltages of 6.44 V

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In this work, we have investigated a simple multi-junction method for achieving high Voc in organic solar cells by stacking individual sub-cells on top of each other. The promising Tetraphenyldibenzoperiflanthen (DBP) was employed as electron donor and Fullerene (C70) was employed as electron acceptor, as they display a relatively high Voc for single junction cells. Both materials show broad absorption in the visible region, making them ideal candidate for multi-junction devices, using these molecules as active materials having a recombination layer in between each sub-cell. By using a 10-Fold bilayer structure of DBP and C70, sandwiched between two electrodes, a very high open circuit voltage of 6.44 V was reached for a single device stack with a current density of 0,68mA/cm² and a power conversion efficiency of around 2%. To further optimize the devices towards higher efficiency, we have modeled the performance of each sub-cell, and from that established the ideal thicknesses required to obtain charge carrier balance in the devices stack. The work shows a promising method for generating high voltage device stacks from small molecule solar cells.

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Optimizing Vertical Organic Field Effect Transistors

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Organic switchable resistors such as field effect transistors (OFETs) are important to realize future flexible electronic devices. In order to reach the needed switching speeds (e.g. for logic applications) and current densities (e.g. for display pixel driving) it is most important to overcome the low charge carrier mobilities and large channel lengths. In this sense, optimizing the geometry is a key element which is done by the novel approach of vertical organic field effect transistors (VOFETs). Here, the vertical channel length where the electric field driven charge carrier drift takes place can easily be scaled down into the sub 100 nm regime. However, a lateral charge diffusion component limits scooping the full potential of the short vertical channel length which is accesible in this device geometry.

Here several approaches to surmount this difficulty are presented.

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Photoinduced resistive switches in hybrid organic structures including colloidal CdSe nanocrystals

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Development of composite structures is an important direction in organic electronics. It was shown in our previous work that composite materials have high potential for memory applications [1]. The operation principles of resistive memory presume an ability of the system to switch between at least two states "ON" and "OFF" with different resistances (resistive switches RS). Embedding metal particles (linear size $\sim 5 \mu\text{m}$) into isolating in pristine state polymer results in RS speed less than 15 ns, non-volatile characteristics, on/off ratio over 2 orders of magnitude, switching electric field below breakdown values, number of rewriting cycles 10⁵ or higher. Samples can be fully fabricated by printing techniques, and we demonstrated that there are no significant differences in their performance compared to samples on hard substrates [2].

For practical application further investigations of downsize scaling impact are required. Replacing metal micro particles with organic photoactive semiconductor particles of various sizes (1.3-2.3 nm in length and 0.3-0.8 nm height) allowed us to control switching voltage using external light source [3]. Introduction of inorganic nanoparticles (NP) can lead to increase in photoresponse and stability of RS in composite structures due to charge transport between NP and organic media.

In this work we observed RS in composite structures consisting of polystyrene matrix with incorporation of colloidal nanoplates CdSe, tert-butyl-substituted lutetium diphthalocyanine, hexadecachloro-substituted lutetium triphthalocyanine and other dyes. We obtained similar results for coplanar and sandwich contact geometries. I-V curve in "OFF" state is attributed to Richardson-Schottky or Poole-Frenkel conduction mechanisms. In "ON" state I-V curve can be approximated by linear ohmic dependence, temperature dependence of conductivity demonstrates metallic type. RS is dependent on external illumination. Photoconductivity spectrum for composite structures demonstrates the same local maximums and minimums as absorption spectrum of NP that confirms charge transport between NP and organic media. We demonstrated that incorporation of CdSe nanoplates into organic matrix provides a promising material for construction of high density and efficient memory.

This work was supported by RFBR (project nb 16-07-00961, 15-03-05890, 16-33-60005).

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Reactivity of LuPc2 thin films towards oxygen

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Lutetium bis-Phthalocyanine thin films are gaining attention as candidate for efficient gas sensing applications. Their peculiar electronic structure, and in particular the presence of a Single Occupied Molecular Orbital (SOMO) makes them ideal candidates for different gas sensing, as they are available for both oxidation and reduction. However no fundamental studies exist yet about how the bonding takes place at the molecular level. In this work we studied the low temperature reactivity towards molecular oxygen of a thick film of LuPc2 deposited on Au(111) single crystal in ultra-high vacuum (UHV). We characterized the reaction via X-Ray Photoelectron spectroscopy (XPS) and Near Edge X-ray Absorption Fine Structure (NEXAFS) spectroscopy. We showed a weak interaction, as oxygen desorbs as the sample is heated up to around 100K. We also showed that the reaction mostly affects the isoindole N atom, and only slightly the C atoms and the π system. We also show that the adsorption geometry is almost vertical. Also quantitative analysis showed that more than a ML was adsorbed, showing the possibility for the oxygen to diffuse inside the layer.

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Solid State Packing Control in Materials for Solar Cells

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Diketopyrrolopyrroles (DPPs) are promising building blocks for organic electronics in general due to their optical properties, good thermal and photochemical stability, good electron affinity for tuning the frontier energy levels, and excellent planarity for enhancing intermolecular interactions and increasing charge carrier mobility [1] DPPs have huge chemical versatility [2] which makes them easy to incorporate in various materials or to be exploited as small molecules for molecular and supramolecular materials, and consequently used for photovoltaic applications [3].

This work presents thiophene based DPP chromophores whose structure and stereochemistry are defined to ensure high specificity in intermolecular interactions in the solid state. These specific functions are addressed through the nitrogen atom and the aromatic rings of the DPP core to control the solubility of the molecule and the packing of the material, and ultimately improve the electron transport and charge collection. Insights of the electronic properties of those chromophores were obtained by solution and solid absorption spectroscopy, cyclic voltammetry and spectroelectrochemistry. Studies in solid state *via* single crystal X-ray diffraction shows unique organisation of the molecules driven by intermolecular hydrogen bonding, as well as important changes in the geometry of the molecule due to other intra- and inter-molecular interactions.

Acknowledgement: We thank Stephen Davies for the electrochemistry and spectroelectrochemistry, William Lewis for single crystal X-ray diffraction measurements and the EPSRC for funding of this research.

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Synthesis and properties of graphene quantum dots and nanomeshes

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We chose to adopt a bottom-up approach for the synthesis and the study of the optical and electronic properties graphene quantum dots (GQDs) and graphene nanomeshes (GNMs) (regular patterns of holes in 2D graphene sheets). The interest of these graphene materials is multiple: the size, morphology and composition of GQDs will influence their electronic properties (as for inorganic QDs). For example, graphene quantum dots exhibiting luminescence in the red or near-infrared region (at wavelength in which living tissues are transparent) may find application in biology. Similarly, by controlling the structure, one can think about reaching $1.5\mu\text{m}$ of emission wavelength (telecom wavelength). The 0D electronic structures of these objects may lead to the emission of single photons at these wavelengths. In this view, it is of high interest to investigate the potentialities of graphene quantum dots. The bottom-up synthesis of 2D networks of graphene containing holes or doping element has not been accomplished so far. In our approach we want to combine theory and experiment to reach the best compromise between the size of holes and their distribution in 2D nanomeshes.

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Thermoelectric characterization of doped organic semiconductors

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The introduction of p- and n-doped layers into the device architecture of organic optoelectronic devices can greatly improve their performance. Charge carrier extraction or injection from or into the organic photo-active layer is enhanced by doping, resulting in a reduction of ohmic losses. Hole and electron selective layers can be realized by molecular doping of organic host materials moving the Fermi level to the appropriate position, enabling electron or hole selectivity. In this work, we use thermovoltage (Seebeck effect) and temperature-dependent conductivity measurements to determine the dominating type of charge carriers introduced by the dopant and to gain insight into the position of the transport level with respect to the Fermi level. The investigation of fullerene dopants with a high degree of fluorination in various amorphous host materials allows us to tune the energy level offset between host and dopant and to study their influence on Fermi level position and overall doping efficiency systematically. We find that even low HOMO materials can be doped efficiently by highly fluorinated fullerenes. Moreover, we observe a clear influence of the energy level offset between matrix and host on the thermoelectric properties and the conductivity. This work provides guidelines for future dopant-matrix combination with a maximum doping efficiency.

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Understanding the charge-transfer state properties in DBP-C70 organic solar cells by means of sensitive external quantum efficiency (sEQE) and morphological studies

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Organic solar cells (OSC)s have attracted research attention during the past years due to their potential advantages as compared to conventional inorganic solar cells [1]. These advantages include low fabrication cost, lightweight, semi-transparency and mechanical flexibility. Despite these advantages, OSCs have comparably low power conversion efficiencies and rather short lifetimes, which put a barrier between laboratory achievements and industrial scale requirements. Therefore, in order to close this gap and to obtain further improvements in the device performance, a detailed understanding of the device working mechanism is required. Charge transfer (CT) states, representing intermediate states between exciton dissociation and recombination at donor-acceptor interface, play hereby a crucial role.

In this work, we study CT states in DBP/C70 based OSCs as a less studied case for inverted and conventional structures. Results from electroluminescence (EL) and sensitive external quantum efficiency (sEQE) measurements show an unexpected difference in charge transfer state energies for each of the two common structures. Moreover, we observe different values for the reorganization energy, which determines the energy loss upon deformation of the molecule during charging. These results suggest morphological sensitivity of the D/A interface, depending on the deposition sequence, which is investigated amongst others by means of atomic force microscopy studies.

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Vertical Organic Light Emitting Transistors for Investigation of Charge Transport in Vertical Organic Field Effect Transistors

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The vertical organic field effect transistor (VOFET) offers many technological advantages due to its very short geometric channel length. However, in contrast to the standard lateral organic field effect transistor (OFET), the basic physics and working principles are not yet well known. In this contribution, we investigate how and where in the device the channel forms, and how different parameters influence the channel. We compare results regarding the charge transport obtained from simulations with measured charge carrier density distributions. The latter ones are obtained from the light emission of vertical organic light emitting transistors (VOLETs). These devices are a combination of an organic light emitting diode (OLED) and a VOFET, which allow to locally resolve the current path via light emission. We show the dependence of the channel size and geometry on several parameters: the gate-source voltage, the drain-source voltage, and the source geometry, and compare them with the simulation data. The active area that contributes to the charge transport, determined by the so called channel depth, increases with higher gate-source voltage. The dependence on the drain-source voltage is more complicated. We give a first characterization based on the standard transistor output equations. A description of the charge path creation inside the vertical device is obtained. A better understanding of the basic phenomena of charge transport in such devices will grant new possibilities for further optimization and improvement.

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- Sancini Giulio
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- Sawatzki Michael
- Sebti Dalia
- Shahini Sharif
- Sherafatipour Golnaz
- Siaugue Jean-Michel
- Sinani Uljan
- Singh Stuti
- Sobolewska Elzbieta
- Tortech Ludovic
- Ugolotti Aldo
- Vitali Michele
- Witkowski Nadine
- Yu Zhe
- Zucca Gaia