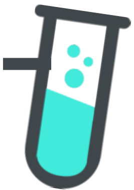
Small Chem

International Online Conference

February 17-18, 2021



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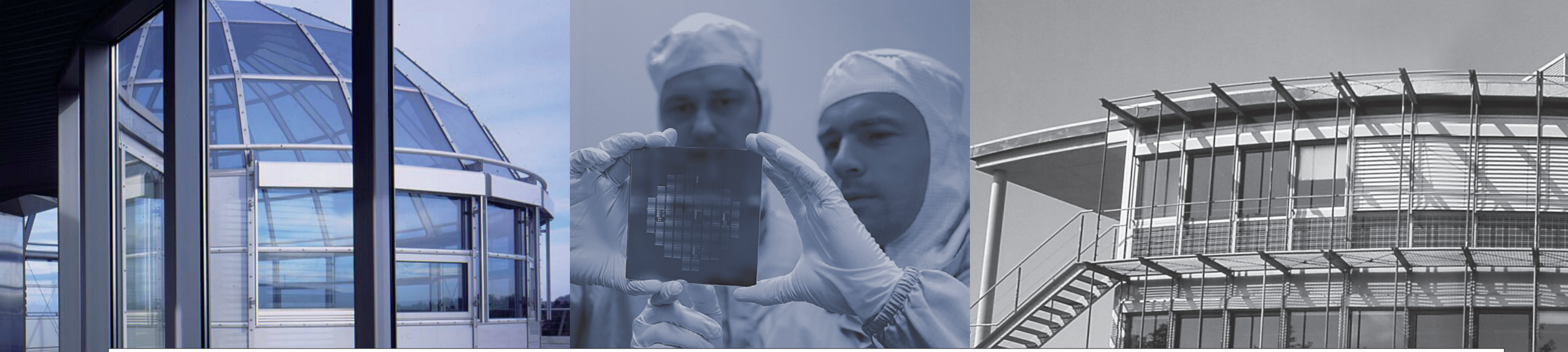

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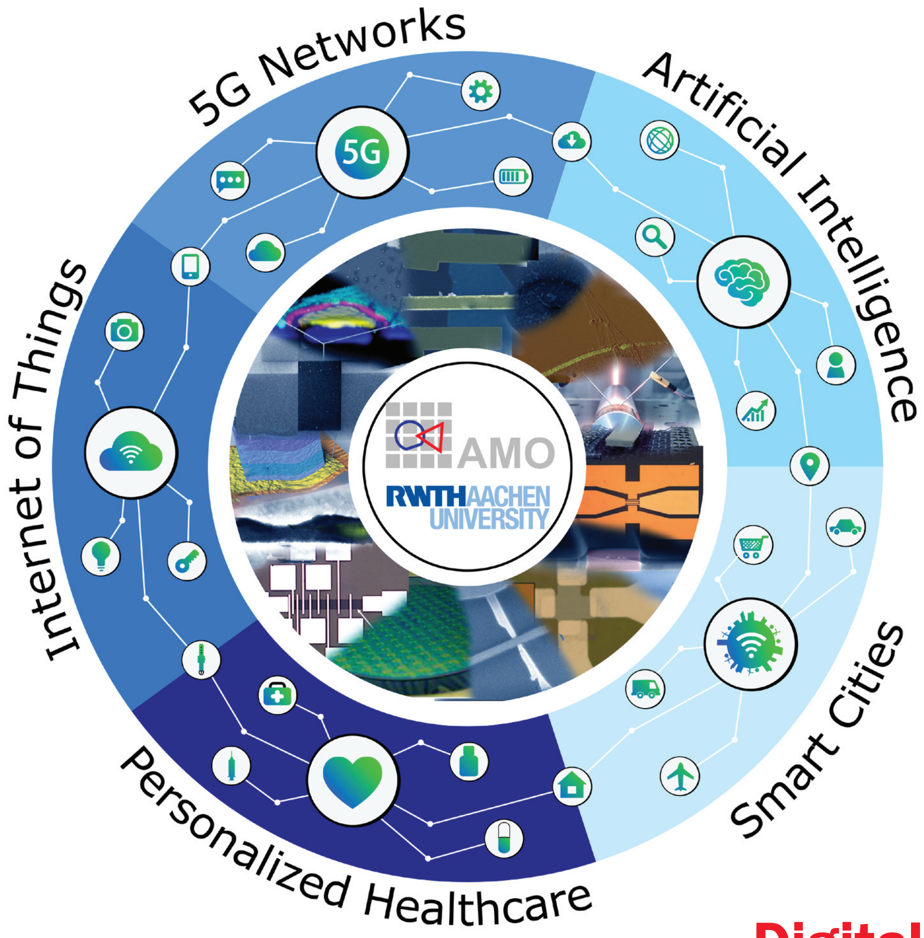

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FOREWORD

On behalf of the Organising and the International Scientific Committees we take great pleasure in welcoming you for the 1st edition of the Small Chem Online International Conference.

Small Chem 2021 will present the most recent advances in fundamental research, technology developments and business opportunities in the Chemistry sector. More than 20 high profile talks from worldwide most influential academia & industry experts will present speeches in this international event on how chemistry latest advances will impact positively our daily life. Small Chem 2021 will be a two-day online event that means to gather the key players of the Chemistry community and related sectors. This event is launched considering that all major scientific and technological in-person conferences are being cancelled or postponed worldwide until middle of 2021.

We are indebted to AMO GmbH (Germany) for their financial contribution and to Merck/Sigma-Aldrich and nanomaterials (MDPI Open Access Journal) for their support.

We also would like to thank all the speakers and participants that join us this year.

Hope to see you again online in the next edition of Small Chem online.

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AMO GmbH is a German high-tech company that acts as a pathfinder for new technologies and as fabrication-service provider in the field of nanotechnology since more than 20 years.

AMO operates a state-of-the-art clean room with advanced nanostructuring capabilities (UV-Nanoimprint, E-Beam lithography, Interference Lithography), offering research and fabrication services that go from proof-of-concept demonstrators to final technological solutions. Main fields of expertise are nanoelectronics, photonics, sensor technology, as well as graphene and other two-dimensional materials.

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KEYNOTE

2D materials beyond graphene: preparation, functionalization and their applications

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Two-dimensional (2D) materials (2DMs), which can be produced by exfoliating bulk crystals of layered materials, display unique optical and electrical properties making them attractive components for a wide range of technological applications. In this context, attaining a full control over the generation of high-quality 2DMs with methods that can be employed for large-scale production of exfoliated nanosheets and inks thereof represents a major challenge of potential technological interest in the numerous fields, even beyond opto-electronics and sensing, such as those associated to energy applications. During this lecture the most recent developments in the production of high-quality 2DMs based inks using liquid-phase exfoliation (LPE) will be discussed,[1] combined with the patterning approaches, highlighting convenient and effective methods for generating materials with controlled thicknesses down to the atomic scale (see Figure 1).

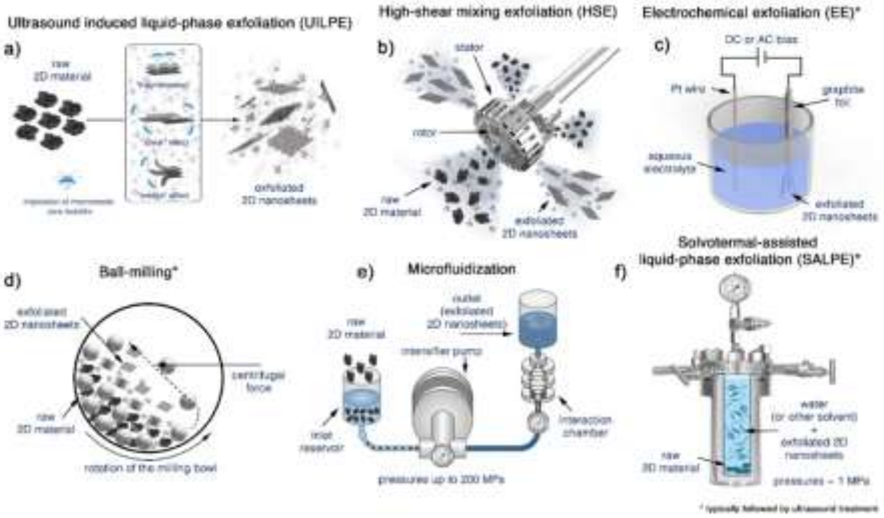

Figure 1: Schematic representation of various liquid phase exfoliation (LPE) based methods such as a) ultrasound induced LPE (UILPE), b) high-shear mixing exfoliation (HSE), c) electrochemical exfoliation (EE), d) ball milling, e) microfluidization and f) solvotermal-assisted LPE (SALPE).

Different processing strategies which can be employed to deposit the produced inks as patterns and functional thin-films will be introduced, by focussing on those that can be easily translated to the industrial scale such as coating, spraying and various printing technologies. By providing insight into the multiscale analyses of numerous physical and chemical properties of these functional films and patterns, with a specific focus on their extraordinary electronic characteristics, this lecture will offer crucial information for a profound understanding of the fundamental properties of these patterned surfaces as the millstone towards the generation of novel multifunctional devices.
The functionalization of 2DMs allows to create foams and coatings integrating novel functions, which comes from the intrinsic design of the molecular units. The second part of this lecture will be devoted to functionalization and the practical use of 2DMs. In particular, molecule–graphene hybrid materials for sensing applications [2] and energy storage [3] will be discussed.

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Molecular magnetism in 2D materials: From chemical design to spin control in molecular devices

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Until recently magnetism has been an elusive property in 2D materials. In this talk the impact of molecular magnetism in this field will be presented [1]. In the first part I will focus on the design of molecular 2D magnets that, in contrast to what happens with the inorganic 2D magnets, are chemically stable in open air, keeping their magnetic properties preserved upon functionalizing their surface with different organic molecules [2]. In the second part I propose to create hybrid heterostructures by interfacing a layer of a functional molecular material with a 2D material. The aim is that of tuning the properties of the “all surface” 2D material *via* an active control of the hybrid interface [3]. To reach this goal the molecular system of choice will be based on spin-crossover complexes able to switch between two spin states upon the application of an external stimulus (temperature, light or pressure). This concept will provide a new class of stimuli-responsive molecular/2D heterostructures, which may be at the origin of a novel generation of hybrid materials and devices of direct application in highly topical fields like electronics, spintronics or molecular sensing.

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Polymer Chemistry in 2D Flatlands

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Abstract

Over the last decade, the discovery of graphene has triggered a new paradigm of two-dimensional (2D) materials. They are featured with a periodic network structure and topographical thickness at the atomic/molecular level, enabling the investigation of fundamental physical and chemical properties down to a single-layer nanosheet. Thereby, robust technologies and industrial applications, ranging from electronics and optoelectronics to energy storage, energy conversion, membrane, sensor, and biomedicine, have been inspired by the discovery and exploration of such new materials.

How can the polymer chemistry contribute to the world of 2D flatlands? In contrast to the tremendous efforts dedicated to exploring graphene and inorganic 2D materials such as metal dichalcogenides, boron nitride, black phosphorus, metal oxides, and nitrides, there remains much less development on organic 2D material systems, including the bottom-up organic/polymer synthesis of graphene nanoribbons, 2D metal-organic frameworks, 2D polymers/supramolecular polymers as well as the supramolecular approach to 2D organic nanostructures. One of the central chemical challenges is realizing a controlled polymerization in two dimensions under thermodynamic/kinetic control in solution and on the surface/interface. This lecture will present our recent efforts on the bottom-up synthetic approaches towards novel crystalline organic 2D crystals with structural control at the atomic/molecular level. We will introduce a surfactant-monolayer assisted interfacial synthesis (SMAIS) method, which is highly efficient to promote precursor monomers' supramolecular assembly on the water surface and subsequent 2D polymerization in a controlled manner. 2D conjugated polymers and coordination polymers belong to such materials classes. The unique structures with possible tailoring of conjugated building blocks and conjugation lengths, adjustable pore sizes and thicknesses, as well as impressive electronic structures, make them highly promising for a number of applications in electronics and spintronics. Other application potential of organic 2D crystals will also be discussed.

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Photocatalytic activity of microporous, structured graphitic carbons

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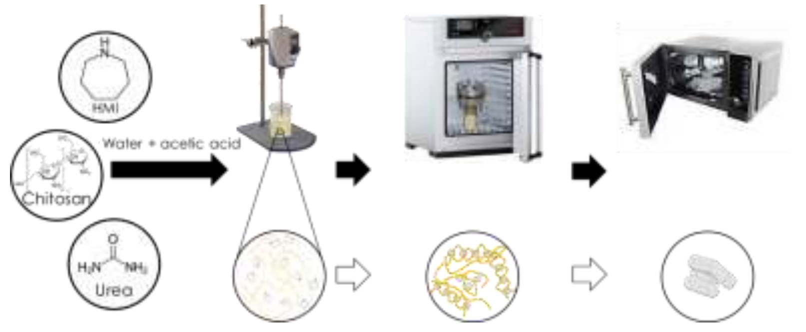
The most frequent photocatalysts contain metals, commonly some that are considered as critical raw materials, such at titanium. For the sake of sustainability there is an increasing interest in developing metal-free photocatalysts that can be obtained from biomass for the conversion of sunlight into fuels and chemicals. In the presentation, it will be described the use of oligo-/poly- saccharides to obtain structured graphitic carbons. Some of them, as those derived from chitosan using templating agents or from cyclodextrins without templation can be converted by pyrolysis in highly crystalline graphitic carbon residues [1]. Scheme 1 presents the concept of the synthesis of one of these materials, while Figure 1 shows a high-resolution TEM image of other material. These carbon residues exhibit regular (ultra)microporosity of subnanometric dimensions. In addition, these materials can be doped with heteroatoms such as N or P. By controlling the composition and structure of these carbons it is possible to influence the properties and activity of these materials.



Scheme 1. Pictuorial illustration of the preparation of microporous graphitic carbon from chitolsan by soft templation

It will be shown that these graphitic exhibit photocatalytic activity under simulated sunlight illumination to promote overall water splitting into hydrogen and oxygen in stoichiometric amounts. The materials appear as stable and reusable under the conditions of the irradiation (Fig. 2).

Overall these studies show how low value biomass wastes can be converted into useful materials that can exhibit important properties and applications, such as for hydrogen generation from water. Thus the results to be presented are a clear case of valorisation of residues and sustainability.

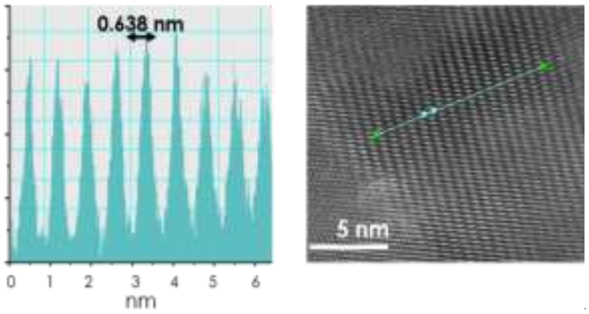


Fig. 1 TEM image of microporous graphitic carbon derived from a-cyclodextrin and periodicity along the green line corresponding to the channel dimension.

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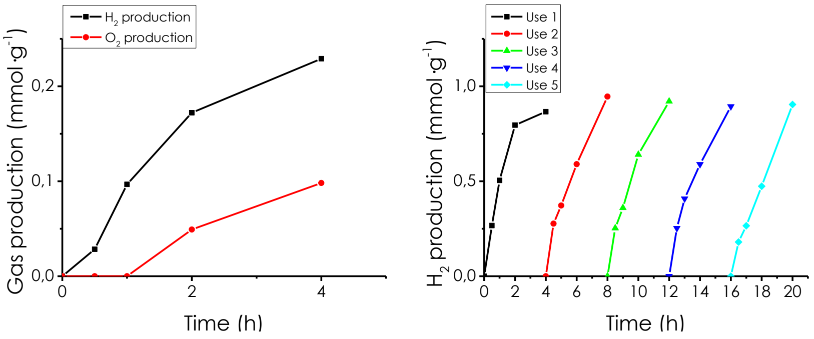

Fig. 2. Temporal profiles of H_2 and O_2 generation upon irradiation with simulated sunlight (1 Sun power) an aqueous suspension of graphitic carbon (1 mg/ml) at ambient temperature. Right: H_2 evolution upon consecutive irradiations under the previous conditions.

Polyoxometalates: from Inorganic Chemicals to Energy Materials

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Polyoxometalates (POMs) are a large and still growing family of inorganic clusters which were thoroughly studied and understood in Inorganic Chemistry labs throughout the world during the second half of the 20thCentury.[1] They are perfect models of quantum-sized metal oxides [2-3] and as such present multiple and interesting properties at the molecular level which can be related to analogue extended systems. Yet, their only target application was, for many years, as catalysts.
Our group was a pioneer in putting polyoxometalates to work as energy-storage materials as it will be presented in this conference. This was achieved by integrating these electroactive clusters in conducting matrices, from conducting polymers [4-5] to nanocarbons [6-8]. The results are striking and show a synergic behaviour that has led to polyoxometalates to be used in prototype electrodes for batteries and supercapacitors. Indeed, the faradaic electroactivity of POMs, in combination with capacitive materials such as nanocarbons is an ideal combination leading to synergic hybrid materials as will be discussed with various illustrative examples.

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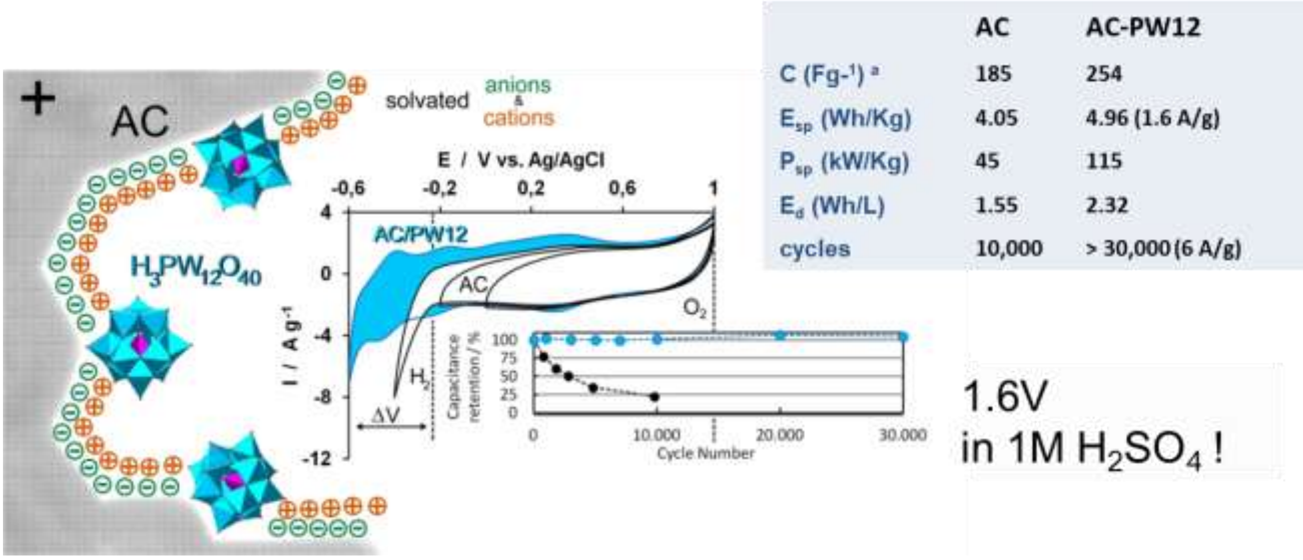
FIGURES



	AC	AC-PW12
C (Fg-^{1}) ^{a}	185	254
E_{sp} (Wh/Kg)	4.05	4.96 (1.6 A/g)
P_{sp} (kW/Kg)	45	115
E_d (Wh/L)	1.55	2.32
cycles	10,000	> 30,000 (6 A/g)

Figure 1: Schematic diagram, electrochemical properties and energy storage performance of a hybrid formed by phosphomolybdic acid (H3PW12O40) and Activated Carbon (AC) (From ref [7])

’Catching the Flu’:
A Supramolecular View on the Interaction of Viruses at Interfaces

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Multivalency describes the interaction between viruses and cell membranes. The influenza virus binds through multiple sialyl-terminated carbohydrates (SLNs) non-covalently interacting with hemagglutinin coat proteins. This interaction is weakly multivalent in nature, and it is expected to be superselective, explaining the large differences between virus affinities by mutations in the receptor binding domain. A key aspect of the multivalent interaction of viruses at cell membranes is its strong dependence on the receptor density displayed at the surface. Here, we show the use of surface gradients [1] of receptor-modified supported lipid bilayers (SLBs) to visualize and quantify the receptor density dependence in one microscopic image (Figure 1) [2]. The gradients in biotin-functionalized SLBs are visualized by using fluorescently labeled streptavidin, onto which biotinylated SLNs are attached. Images of of dye-labeled influenza viruses binding to these platforms show a steeply, nonlinear dependence of the virus coverage on the SLN density, which is the hallmark of superselective binding. The description of the data by a thermodynamic model allows quantification of the threshold density, comparison of binding selectivities for different virus strains, and a molecular understanding of the supramolecular binding energy landscape. This supramolecular and nanoscopic picture links fundamental molecular aspects of binding to biological processes of antigenic drift and zoonosis.

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FIGURES

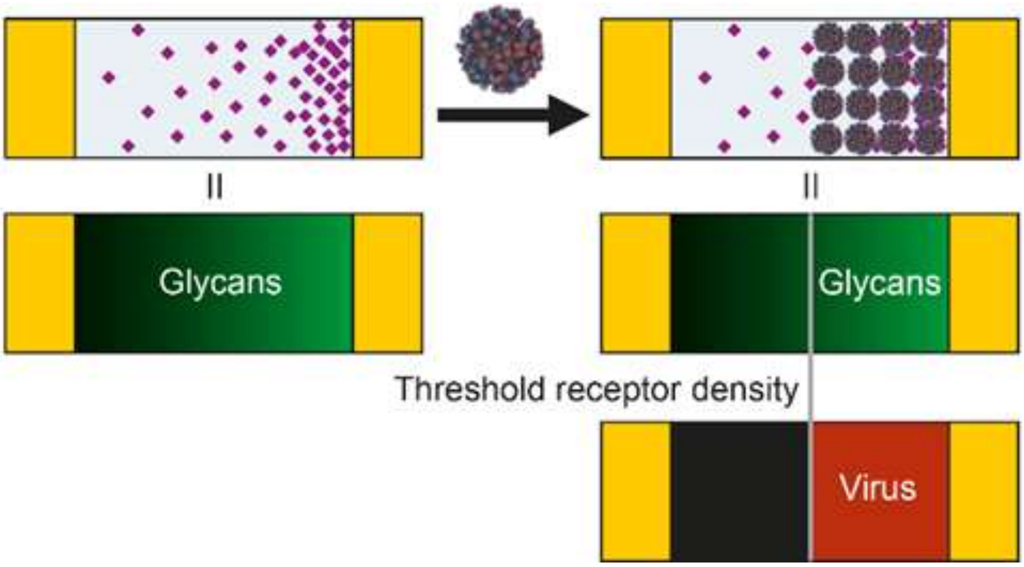

Figure 1: Concept of using receptor-modified surface gradients as a way to detect the threshold receptor density of a virus

Additive engineering for stable halide perovskite solar cells

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Abstract

Halide perovskite solar cells (PSCs) have already demonstrated power conversion efficiencies above 25%, which makes them one of the most attractive photovoltaic technologies. However, one of the main bottlenecks towards their commercialization is their long-term stability, which should exceed the 20-year mark. Additive engineering is an effective pathway for the enhancement of device lifetime. Additives applied as organic or inorganic compounds, improve crystal grain growth enhancing power conversion efficiency. The interaction of their functional groups with the halide perovskite (HP) absorber, as well as with the transport layers, results in defect passivation and ion immobilization improving device performance and stability. In this talk, we will briefly summarize the different types of additives recently applied in PSC to enhance not only efficiency but also long-term operational stability. We discuss the different mechanism behind additive engineering and the role of the functional groups of these additives for defect passivation. Special emphasis is given to their effect on the stability of PSCs under environmental conditions such as humidity, atmosphere, light irradiation (UV, visible) or heat, taking into account the recently reported ISOS protocols. We also discuss the relation between deep-defect passivation, non-radiative recombination and device efficiency, as well as the possible relation between shallow-defect passivation, ion immobilization and device operational stability. We will also show our most recent results applying additives in PSC where we have been able to obtain efficiencies above 21 % and highly stable devices showing null degradation after more than 10000 h under continuous light irradiation of 1 sun.

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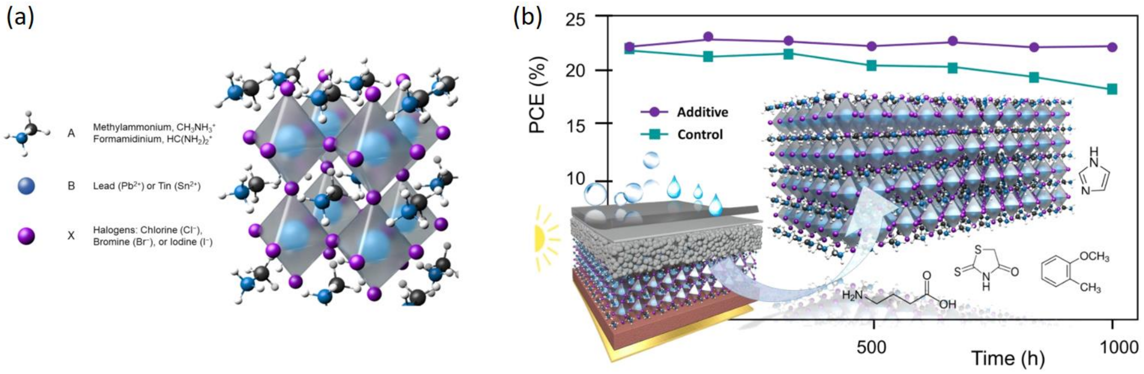

Figure 1: (a) Schematic representation of Halide perovskite structure and (b) the effect of additive engineering on perovskite solar cell operational stability [7].

Spatial organization of multi-enzyme systems in porous materials

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Combination of several enzymes in one-pot opens a very attractive pathway to access more complex synthetic schemes to manufacture high added-value products in a more sustainable manner. Nowadays, chemical biomanufacturing is dominated by microbial fermentations that use native pathways to mainly produce alcohols, acids or aminoacids. In the last decade, cell-free multi-enzyme systems have emerged as an alternative to whole cell biotransformations in chemical manufacturing[1]. However, enzyme isolation faces some challenges (productivity, robustness and costs) for implementing cell-free multi-enzyme systems into the industrial context. Scaling-up cell-free bioprocesses involving cofactor-dependent enzymes are even more challenging because they demand for exogenous cofactors that hamper the downstream processing and limit their economic feasibility of the process. Inspired by the spatial organization and the molecular confinement of metabolic pathways within the living cells, our group has exploited several immobilization techniques to spatially organized a variety of multi-enzyme systems (oxidoreductases, oxidases, transaminases) confined with their corresponding cofactors (NAD(P)H, PLP, FAD…) across the surface of synthetic porous carriers[2,3]. Our work aims at creating in vitro and confined enzymatic pathways as self-sufficient and multi-functional heterogeneous biocatalysts, where cofactors and enzymes are successfully recycled and reutilized during several operational cycles to increase their total turnover numbers (TTN). The performance of these immobilized multi-enzyme systems has been expanded to flow-biocatalysis and accompanied by some metrics that quantify the sustainability of the processes.

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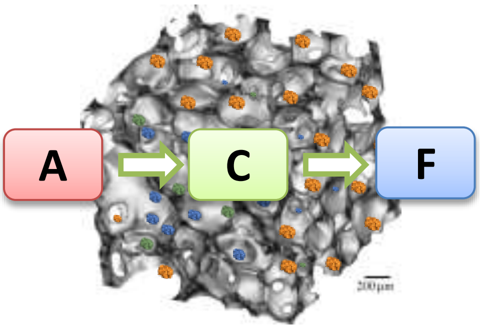

Figure 1: Spatial organization of enzymes across the porous surface of solid carriers for step-wise biocatalysis

Metal clusters of small atomicity synthesized by kinetic control with outstanding physicochemical properties

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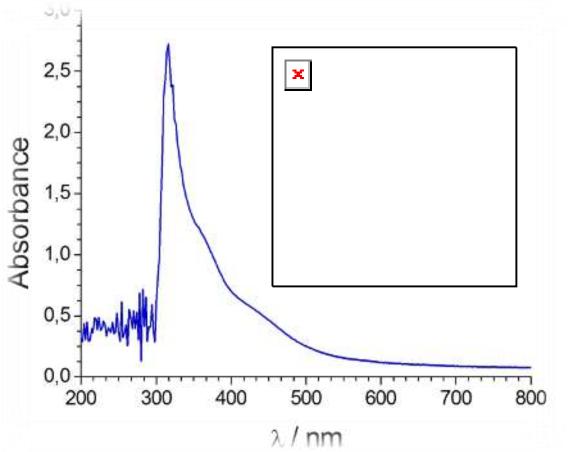
Typical metal nanoparticles show scaling behavior properties. However, when particle size is reduced below ≈ 2 nm (clusters of atoms) quantum confinement break the scaling laws and the properties of metal clusters become dramatically different from the nanoparticles [1].
In general, clusters can be divided into (i) large clusters –consisting of a core formed by a number of metal atoms in the number range ~10-20 to 10-200 atoms and a protecting shell of strong ligands such as phosphines or thiols and (ii) small clusters – formed by a small number of atoms ~2 to 10-20, which - contrary to what is commonly assumed- do not need any strong stabilizing ligand and have almost all of their atoms on the surface [1]. We will show here that such small clusters can be synthesized *wet chemical techniques* without using binding ligands. The key point to achieve the preparation of such "naked" clusters is the use of the *kinetic control method* [2]. Using such method our research group has synthesized very monodisperse clusters of different metals (mainly Ag, Au, Cu and Pt), with sizes in the range 2 to ≈ 30 atoms [3]. As an example, we show in Figure 1 (left) the UV-Vis absorption spectrum of Au_9 clusters (the inset shows for comparison the plasmon band of Au nanoparticles). It can be seen that the absorption is similar to semiconductors and this similar behavior can be used to get information of the cluster's size. Figure 1 (right) shows the corresponding Tauc plot, indicating that such clusters behave as a direct-like semiconductor with a bandgap (HOMO-LUMO gap) = 2.6eV. Taking into account the Jellium model this gap would should correspond to a cluster with N=9 atoms [$N=(E_F/E_g)^3=(5.4/2.6)^3=9$]. We will also report here some of their exceptional physicochemical properties, mainly in the fields of catalysis [4] and therapeutics [5].



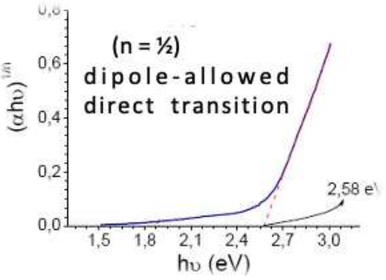


Figure 1: Left: UV-Vis absorption spectrum of Au_9 clusters (inset shows, for comparison, the plasmonic absorption of Au nanoparticles). Right: Tauc plot of the cluster absorption indicating a clear dipole-allowed direct transition (n=1/2).

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Innovative polymers for next generation batteries

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Lithium ion batteries are part of our modern life being present in daily used objects such as mobile phones, tablets, computers, watches, sport accessories, electric scooters or cars. The next generation batteries would need the development of innovative polymers that help to improve their performance in terms of power density, cyclability, raw materials availability, low weight, printability, flexibility, sustainability or security. In this presentation we will discuss our recent developments in the area of redox active and ionic conducting polymers.[1-4] This includes the development of innovative binders for electrodes, polymer electrolytes and redox polymers. All these new polymer developments are leading to new battery technologies such as metal-polymer batteries, organic batteries, polymer-air and redox-flow batteries which are expected to complement in the future the actual commercial batteries.

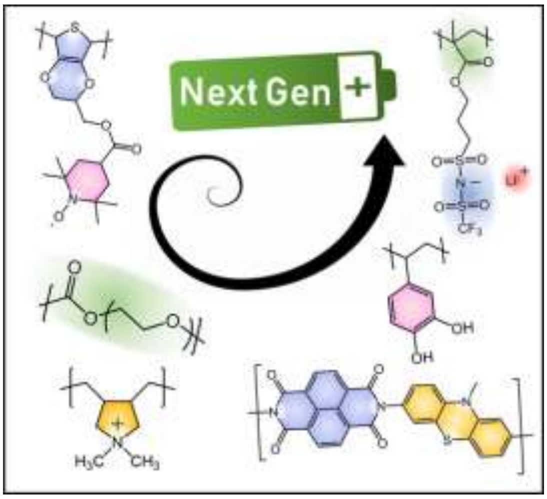

Figure 1: Scheme of some of the polymers will be discussed for application in emerging batteries

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Real-time imaging of Na+ reversible intercalation in “Janus” graphene stacks for battery applications

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Sodium, in contrast to other metals, cannot intercalate in graphite, and this hinders the use of this cheap, abundant element in rechargeable batteries. Here, we report a nanometric graphite-like anode for sodium ions storage, formed by stacked graphene sheets functionalized only on one side, termed Janus graphene. The asymmetric functionalization allows reversible intercalation of Na^+, as we monitored by *operando* Raman spectro-electrochemistry and visualized by imaging ellipsometry, both in real time. Our Janus graphene has only one chemical functional group, uniform pore size, controllable functionalization density, very few edges; it can store Na^+ differently from both graphite and stacked graphene. Density Functional Theory (DFT) calculations demonstrate that Na^+ preferably rests close to the $-NH_2$ group forming a synergic ionic bond to graphene, making the interaction process energetically favourable. We estimate a sodium storage up to $C_{6.9}Na$, comparable to what currently achieved in standard lithium ion batteries. Our approach provides a new concept to design carbon-based materials as anode for the application of sodium ion battery.

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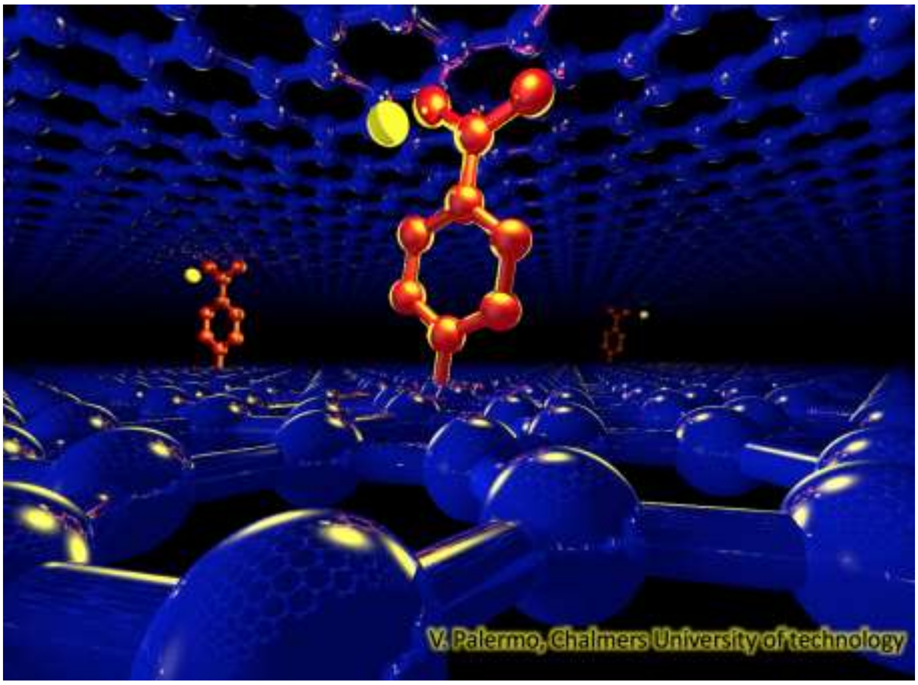

Figure 1: Cartoon showing Na+ ions intercalated in between graphene sheets with aminobenzene spacers.

Molecular Approaches to Energy Conversion

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During my lecture I will present our latest results[1,2] on the characterization of different type of solar cells from DSSC and OPV to MAPI using advanced photo-induced time resolved techniques. Using PICE (Photo-induced charge extraction), PIT-PV (Photo-induced Transient PhotoVoltage) and other techniques, we have been able to distinguish between capacitive electronic charge, and a larger amount of charge due to the intrinsic properties of the perovskite material. Moreover, the results allow us to compare different materials, used as hole transport materials (HTM), and the relationship between their HOMO and LUMO energy levels, the solar cell efficiency and the charge losses due to interfacial charge recombination processes occurring at the device under illumination. These techniques and the measurements carried out are key to understand the device function and improve further the efficiency and stability on perovskite MAPI based solar cells.

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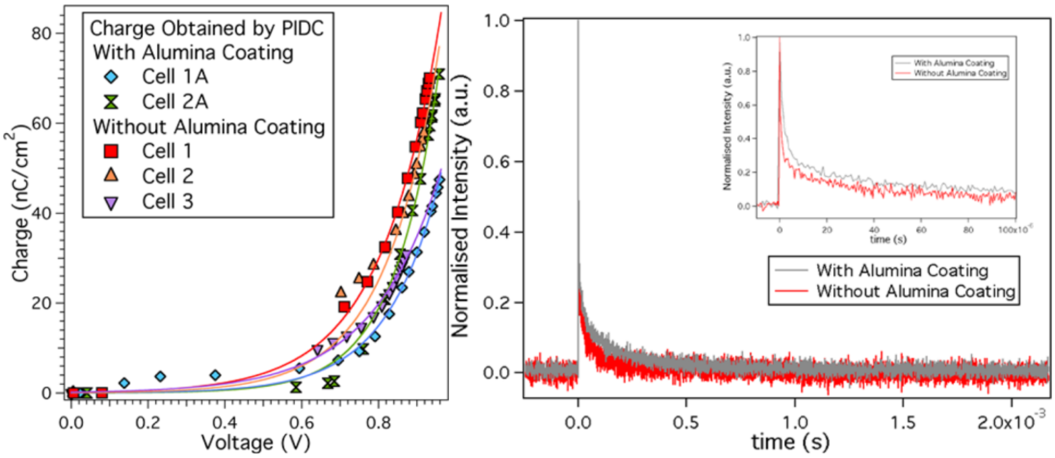

Figure 1. Measured charge in complete devices (left) using PIDC (Photo Induced Differential Charging) and the measured PIT-PV (Photo Induced Transient Photovoltage) decays for two solar cells with different TiO2/MAPI interface.

Chemically-Fuelled Non-Equilibrium Self-Assembly

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Nature extensively exploits transient self-assembly structures with high energy that are able to perform work through a dissipative process. Often, self-assembly relies on the use of molecules as fuel which is consumed to drive thermodynamically unfavourable reactions away from equilibrium.[1] Implementing this kind of non-equilibrium self-assembly processes in synthetic systems is bound to profoundly impact the fields of chemistry, materials science and synthetic biology leading towards innovative dissipative structures able to convert and store chemical energy.

Here, I will present recent contributions by our group that show how ATP can be used as a chemical fuel for the transient self-assembly of vesicles.[2-5] These vesicles act as nanoreactors for chemical reactions, which are transiently upregulated when ATP is added. We will also show that a hydrogel containing catalytic nanoparticles can be maintained in a stationary non-equilibrium state upon local UV-irradiation causing an enhanced catalytic activity as a result of persistent concentration gradients in the gel.[6]

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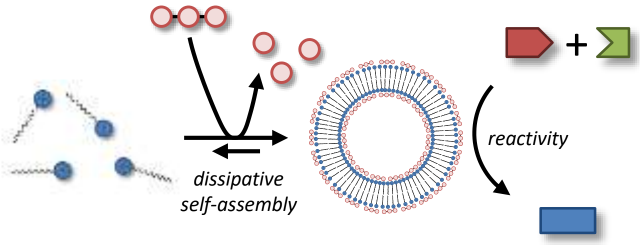

Figure 1: ATP-fueled transient self-assembly of vesicular nanoreactors [3]

Zeolite design for selective adsorption and separation processes

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Gas separation processes need of complex infrastructures and are highly demanding of energy [1]. This is the case of two particular gas separation processes. i) Natural gas upgrading in which CO2 must be removed prior to be transported, either as liquid or through pipelines [2] and ii) olefin recovery from C2 and C3 raffinate streams coming from the steam cracker [3].
These two separations are highly challenging and of huge economic impact since the first could be of interest for small natural gas resources, while the second could avoid of the cryogenic distillation units used in current refineries.
The particular necessities of these two separations are nice examples for showing how properties of zeolites (or any adsorbent) can be tailored for maximizing the production of the separation units at the lowest energy demand.

First, the influence of pore aperture and channel dimensionality and chemical composition in the adsorption capacity and gas selectivity for upgrading of Natural Gas was studied. It has been found that zeolites of relatively low micropore volume to surface area ratio give a better performance for CO_2/CH_4 separation. Also, the chemical composition of the zeolite influences the polarity of the adsorbent, being of paramount importance for effective CO_2/CH_4 separation [4]. Additionally, cation gating effect occurs and relocation of compensating cations reduces the effective window opening for gas diffusion [5,6].

Secondly, we show the applicability of pure silica zeolites for olefin separations, since the lack of any acid site avoid the pore blocking due to olefin oligomerization inside the void volumes of zeolites. The rational selection of the adequate zeolite structure maximizes the adsorption capacity of the desired olefin [7-9]. Finally, it will be show how very tiny modification in the pore opening could have a dramatic influence into the selectivity during competitive adsorption processes [10,11].

These results exemplify which are some of the parameters governing adsorption processes and the strategies taken for improving productivity and selectivity during gas separation processes.

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Multimodal polymeric nanocapsules for imaging and therapy. Application to neurorepair.

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A key challenge in nanomedicine, especially in difficult-access tissues such as the brain, is the non-invasive administration of nanocarriers and the controlled release of their therapeutic cargo. New biocompatible formulations for *in vivo* neuroimaging monitoring are necessary during pre-clinical research phases. I will present some chemical routes to attain theranostic poly(lactic-co-glycolic acid) (PLGA) nanocapsules incorporating "3-in-1" multimodal imaging capacities (MRI, fluorescence at different wavelengths and ^{89}Zr-radiolabeling for PET) and their biodistribution studies [1,2]. The proposed modular synthetic approach allows the simultaneous combination of contrast agents without affecting the size or shape of the nanocapsules, nor interfering with the therapeutic agent.

Those novel polymeric magnetic nanocapsules are proposed for brain tissue imaging and repair in the context of an ischemic event by delivering therapeutic growth factors into the peri-infracted areas [3]. Their engrafting into mouse brain can be assisted by an external magnetic field [4,5]. We expect that in the future, our approach will provide an advanced therapy that could be translated to the clinics as noninvasive, safe, and available to most stroke patients.

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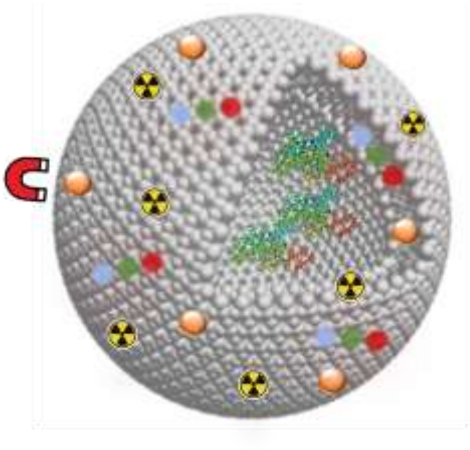

Figure 1: Schematic illustration of a polymeric nanocarrier with imaging probes and therapeutic cargo

INVITED

Tailored electrochemical interfaces for renewable energy conversion

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ABSTRACT

The design and development of active, stable and selective electrocatalysts for energy conversion reactions is key for the transition towards a sustainable future. Investigating the electrochemical interface at the atomic and molecular levels is essential to understand the structure-reactivity relations and tune the active site for electrocatalytic reactions.

This talk will first focus on tailored electrocatalysts for renewable energy conversion reactions such as oxygen reduction and evolution (ORR and OER, respectively). The slow kinetics of the ORR and OER limits the performance of proton exchange membrane fuel cells and electrolysers for the use and production of green hydrogen. I will present our work on oxygen electrocatalysis, from model studies on well-defined surfaces [1,2] to the development of self-supported high-surface area nanostructured catalysts for ORR and OER [3,4] (Figure 1, left).

In the second part, I will discuss about the role of pH, electrolyte anions and structure sensitivity on well-defined Cu electrodes for CO and CO_2 reduction [5] (Figure 1, right). We have studied the effect of pH, anion adsorption, and potential dependence of interfacial processes for CO reduction [6,7]. We show how model studies are essential to understand the structure-property relationships and design efficient electrocatalysts for sustainable energy conversion.

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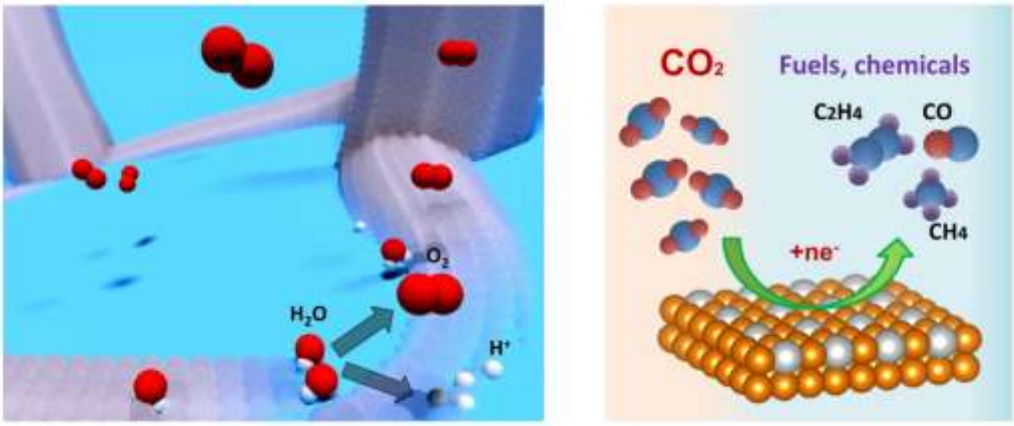

Figure 1: Schematic illustration of Ir nanostructured networks for electrochemical water splitting (left) and Cu-based electrocatalysts for CO_2 reduction to green fuels and chemicals (right).

Advanced materials for a sustainable future

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Global trends such as population growth, climate change, urbanization and an increasing demand for energy are major challenges to **future mobility concepts**. Energy management is a specific challenge for all the vehicles and **materials design** can be considered a key enabler of smart, green and integrated transport. This “green motoring” implies not only alternative propulsion systems but also lightweight materials to reduce the amount of energy needed to start the vehicle besides, performance improvements, operation costs optimization and flexibility. In this context, two examples of key technologies and materials are reviewed in detail. Lightweight materials as a replacement for existing solutions, are essential to improve the energy efficiency of many types of engineering equipment and systems in fields including energy production, transportation and construction. The combination of **cellular materials and nanotechnology** open new areas of opportunity to be explored. On the other side, materials for advanced battery technologies will impact how energy is used and stored at many levels from regional power distribution applications to improved sustainable mobility and new generation electronic consumer goods. One of the solutions to overcome energy density limitations based on **sulfur polymer carbon composites cathode is presented**.

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Electrocatalyst Materials for Sustainable Energy Conversion

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Recyclability and re-use of highly active nanocatalysts [1] is still an outstanding global challenge of increasing importance in the area of energy conversion and heterogeneous catalysis.Electrochemical devices based on electrocatalyst materials containing precious metals, such as Pt, are currently hindered by their short-term durability. As these precious elements are rapidly diminishing, the research community is forced to urgently address this major issue until more abundant efficient electrocatalysts are put forward. In this respect, hollow carbon nanostructures can provide an excellent mean for the fabrication of highly durable electrocatalyst materials through nanocatalyst confinement [2,3], allowing their sustainable use in electrochemical processes. These surprising and remarkable properties of the reported hybrid electrocatalyst materials has opened up a new strategy for the sustainable use of precious metals in electrocatalysis and other technological applications that require stabilization of metal nanoparticles under harsh conditions (Figure 1).

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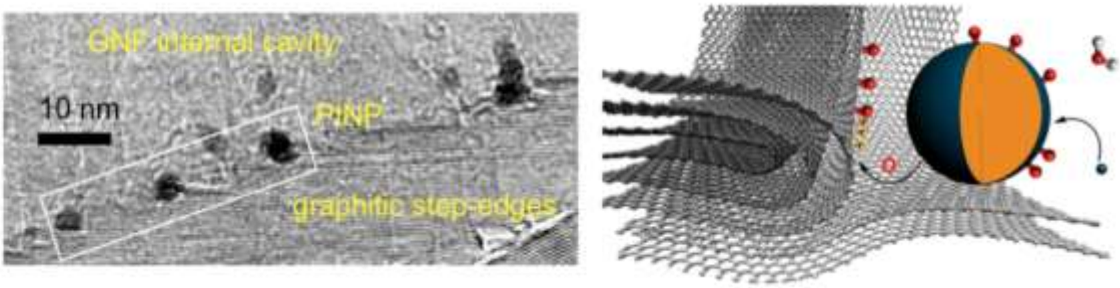

Figure 1: A HRTEM image (left image) and a scheme (righ image) of the internal cavity of a electrocatalytic nanoelectrode with nanoparticles positioned predominantly at the graphitic step-edges.

From Organic Chemistry to Nanoscience:
Studies on Aromatic Compounds.

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Since their interesting theoretical and practical implications, aromatic compounds play a central role in Organic Chemistry, being a frequent structural motif in many chemicals with a variety of appealing chemical, physical, biological and technological properties.
Our group has been involved in the research on many different aspects of aromatic compounds that include the following issues:

a) Synthetic applications of biocatalysis.
b) Non-covalent interactions of aromatic compounds.
c) Towards the quantification of aromaticity.
d) Computational toxicology of aromatic compounds.
e) Peptide-arene hybrids: synthesis, structure and properties.
f) Inhibitors of the protease calpain.
g) Gold nanoparticles ‘decorated’ with peptide-biphenyl hybrids.
h) Aromatic ionic liquids as electrolytes for batteries.
i) Research on graphene.
j) Setting an spin-off.

In the meeting, we will highlight some results on these different topics.

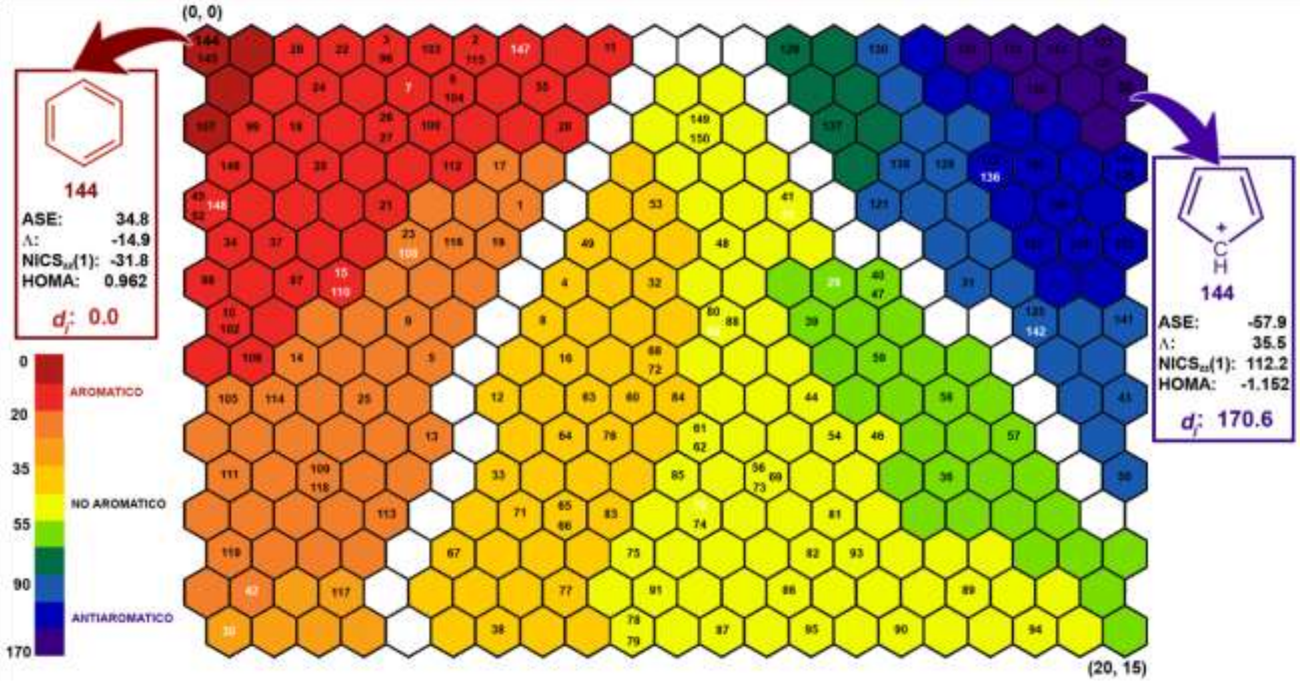

Figure 1: Neural network that classifies organic compounds based on their aromatic, non-aromatic, and antiaromatic characters. The Euclidean distance between neurons (relative to the one activated by benzene, the most aromatic compound) can be used as a quantitative scale of aromaticity.

Photonic Lab-on-a-Chip: Integration of Optical Spectroscopy in Microfluidic Systems

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Photonic lab-on-a-chip analytical systems (PhLoCs) are considered the unique integration of photonic systems with microfluidics. In this seminar, we will discuss the main principles that have paved the PhLoC development, and specially for the on-chip spectrophotometric detection.

The synergistic combination of photonic integrated circuits (PICs) with LoC gives rise to the photonic lab-on-a-chip (PhLoC) concept [1], Therein, the main function of microfluidics is the manipulation and transport of the analytes, while the PICs transduce the (bio)chemical signal arising from the analytes in situ to a quantifiable signal. In this context, the implementation of a PhLoC has to be based firstly on the selection of the appropriate detection mechanism, i.e., colorimetry [2], fluorimetry [3], scattering [4] or plasmonics [5], and secondly, the design of the PhLoC, considering both the optical properties of the materials and the geometry of the optical elements. In this presentation, either monolithic [6] and modular (figure 1) [7] PhLoC concepts will be discussed.

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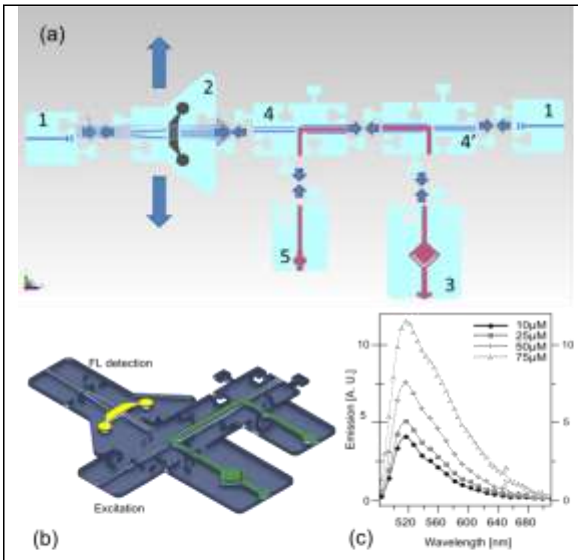

Figure 5. (a) Design-scheme of the modular optofluidic system (MOPS) used in this work. The individual modules are: 1) Two fiber optics connections, 2) a solid/liquid absorbance filter (filled with a colorant or a doped sol-gel) which can be included or excluded as required, 3) a fluidic inlet port with an internal air bubble based pressure regulator, 4/4') two waveguides directed to a microchannel which is shielded with air mirrors to prevent optical cross-talk, 5) a fluidic outlet port; (b) 90º configuration for fluorescence measurements; (c) Emission spectra of aqueous Fluorescein solutions with different concentrations. Figures published at [7] and reproduced by permission of The Royal Society of Chemistry.

Functional self-assembled molecular monolayers for electrochemical devices

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The surface modification of solid inorganic supports with chemically bonded self-assembled monolayers (SAMs) has been proved to be a promising and versatile route for the development of smart surfaces that are able to respond to an external stimulus. In this context, SAMs of electroactive molecules on conductive surfaces offer the opportunity to tune the surface properties by the application of an electrical signal. Alternatively, SAMs with receptor groups that can interact with target analytes promoting an electrical response are also highly appealing for sensing purposes. Here, we will show our work on the preparation of SAMs to be exploited as molecular switches with different electrical, optical or chemical outputs. [1-2] Additionally, some of these SAMs have been exploited for more advanced devices such as for water actuation, of high interest in the field of digital microfluidics (Fig.1).[3] Finally, SAMs have also been implemented into electrolyte-gated organic field-effect transistors (EGOFETs) for both the fabrication of memories and sensing devices.[4-5]

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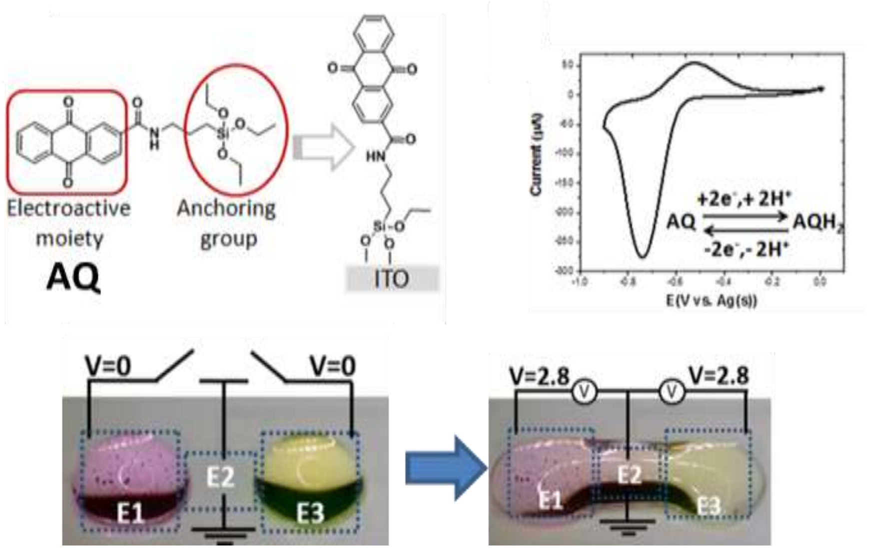

Figure 1: Top: Self-assembled monolayer (SAM) of an anthraquinone (AQ) derivative on indium tin oxide (ITO) with its corresponding cyclic voltammetry showing its redox character. Bottom: Snapshots of the water actuation performed with these SAMs (droplet merging).

Engineered graphene composites for enhanced drinking water purification technologies

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The purification of water from microcontaminants is a major urgent problem worldwide. Much of our tap water comes from rivers, streams, lakes and groundwater. These water resources are increasingly contaminated by discharges of chemicals from industries and urban areas, most of them not fully removed by standard water treatment. Traces of prescription medications, antimicrobial chemicals, pesticides, cosmetics, with suspicious or even proved toxic effects have been found in several EU water bodies. [1] In answer to such crucial issues, the new European Drinking Water Directive EU 2020/2184 [2] includes new limits and contaminants and a water safety plan approach, calling for the urgent development of low cost and efficient water purification technologies. In the last years, Graphene oxide (GO) has shown great potential as adsorbent for water purification from organic microcontaminants, metal ions and heavy metals. [3] The high surface area and the presence of oxygen surface functionalities makes GO particularly suitable for the adsorption of contaminant including those of emerging concern (EC). [4]

Here, we report on GO-polymer based filters, both membranes and sorbent types, for Point-of-Use (POU) drinking water purification systems. We describe the preparation of new polysulfone/polyethersulfone (PSU/PES)-graphene oxide (GO) composites with tuneable surface properties though tailored GO chemical functionalization. We demonstrate the suitability of GO enhanced membranes and sorbents for the fabrication of filters for the removal of emerging contaminants from tap water.

Stable fixation of GO on commercial PSU and PES membranes and granular sorbents was achieved by a water-based procedure under mild thermal activation. Selectivity and filtration efficiency on selected contaminants including very persistent ones such as perfluorinated alkylate substances (PFAS), arsenic and antibiotic, as well as filter working mechanism will be discussed. Particular focus on the relationships between graphene functionalization /surface charge/amount, type of polymeric substrate, with the removal performance will be given.

Figure 1: Tap water purification by graphene composite-based POU filters

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Spatiotemporal control over adhesions of synthetic cells using light

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Many functions in cells arise directly from the spatial and temporal regulation of cell-matrix and cell-cell interactions. [1] In this talk, I will present strategies of how such spatiotemporal control over adhesions of synthetic cell-like systems can be achieved with visible light. These light triggered and reversible interactions mimic the dynamics of interactions observed in biology, and allow modulating the interactions as desired without disturbing other processes in the system.

A prime example for spatiotemporal regulation resulting in function are the adhesions during cell motility. As cells move new adhesions form at the front and adhesions disassemble at the back. To replicate this dynamic and spatiotemporally controlled asymmetry of adhesions and achieve motility in a minimal synthetic cell, we controlled the adhesion of a model giant unilamellar vesicle (GUV) to the substrate with light. For this purpose, we immobilized the proteins iLID and Micro, which interact under blue light and dissociate from each other in the dark, on a substrate and a GUV, respectively. Under blue light the protein interaction leads to adhesion of the vesicle to the substrate, which is reversible in the dark. The high spatiotemporal control provided by light, allowed partly illuminating the GUV and generating an asymmetry in adhesions. Consequently, the GUV moves into the illuminated area, a process that can be repeated over multiple cycles. [2] Thus, our system reproduces the dynamic spatiotemporal distribution of adhesions and establishes mimetic motility of a synthetic cell.

Cell to cell communication is a process that depends on the proximity of a sender and a receiver cells. Similarly, using photoswitchable adhesions between sender GUVs and receiver GUVs we are able to regulate their communication through soluble molecules with light. [3] Overall, our work on one hand provides insight into underlying design principles of life and on the other hand allows addressing questions in cell biology as well as engineer new synthetic cell biology.

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ORALS

Curcuminoids: Molecular Platforms for Electronic and Sensor Purposes

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Nowadays, curcuminoids (CCMoids)[1-9] and related coordination compounds are progressively explored besides biomedicine (e.g.: photovoltaics[2] and MOFs[3]) in additional contributing areas of Nanoscience and Nanotechnology due to their structural nature and versatile chemistry.

During the last years, my group has designed a number of these molecules as metal-anticancer agents,[4] single-molecule magnets[5-6] and coordination polymers.[7] Moreover, their conjugated skeleton and adaptable endings have triggered their study in Molecular Electronics as molecular wires between Au[8] and graphene[9] electrodes. The use of extra functional groups allows their attachment to different surfaces, exploring this way their luminescent properties.

Here, I would like to emphasize our work in the last two topics: (i) single-molecule transport studies of CCMoids using mechanically-controllable break junction technique (MCBJ)[8] and (ii) surface engineering, with the creation of patterns on substrates using micro-contact printing technique (μ-CP). In the former, the combination of a CCMoid, containing methylthio units as anchoring groups and boron coordination promotes electric-field induced bistability in conductance measurements at the single molecule level.[8] The second shows that CCMoids, with fluorophore groups, are capable of functioning as sensors of boron materials acting, in some cases, as NIR fluorescent probes.

Our work emphasizes the potential of CCMoids as molecular key components in electronic devices and sensors owing to their thorough design.

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Optical sensing of spin-crossover compounds with 2D materials

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Abstract

The dimensionality of a system plays an important role on the properties of matter. As an example, the discovery of graphene and its outstanding properties [1] has motivated scientists to continue looking for other two-dimensional (2D) materials that could be comparable or even exhibit better and different properties for a wide range of technological applications. In this context, molecular materials have not been fully studied yet but are strong candidates to observe the proximity effects between molecular and inorganic systems at the 2D limit.

In this work, thin layers of a spin-crossover (SCO) material [2] are obtained through dry mechanical exfoliation. These systems are metal complexes of Fe(II) where the spin state of the metallic center changes between high-spin (HS) and low-spin (LS) upon application of an external stimulus (light, pressure, temperature, voltage…), showing their potential as memory devices or in spintronic applications [3]. They can be combined with inorganic 2D materials to study their synergy in different physical properties, such as their electronic or optical response. In this work, we study the optical properties using Raman spectroscopy and optical microscopy to understand how the polarization of the incident light affects the optical response of the SCO material (Figure 1.a). Moreover, we fabricate van der Waals heterostructures by combining the SCO with monolayers of WSe_2 (Figure 1.b) in order to study the interplay between them.

Our results illustrate the synergy between the SCO and the inorganic system and opens the door to explore further molecular compounds of interest whose properties cannot be detected otherwise.

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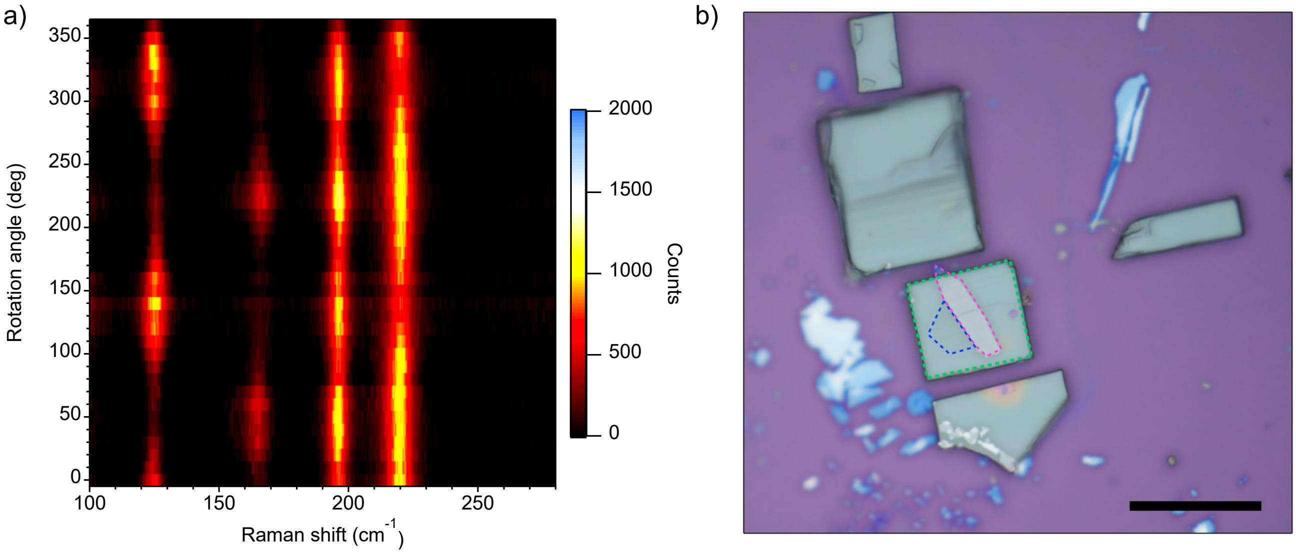

Figure 1: a) Raman spectra of the SCO as a function of the polarization of the laser. b) Optical image of a SCO/WSe_2 van der Waals heterostructure. The dashed lines correspond to the SCO (green) and the WSe_2 (the blue lines for the monolayer; the pink lines for a thicker flake). Scale bar: 20 µm.

Transformation between 2D and 3D Covalent Organic Frameworks via Reversible [2 + 2] Cycloaddition

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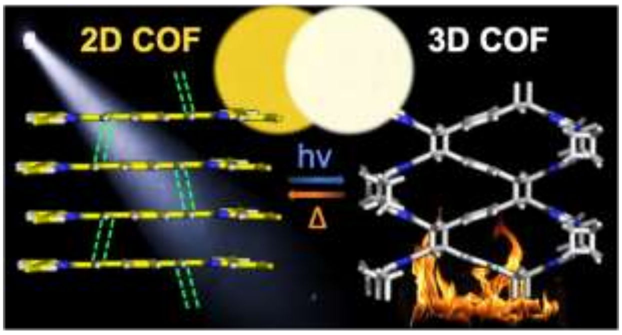
Abstract

We report the first transformation between crystalline vinylene-linked two-dimensional (2D) polymers and crystalline cyclobutane-linked three-dimensional (3D) polymers. Specifically, absorption-edge irradiation of the 2D poly(arylenevinylene) covalent organic frameworks (COFs) results in topological [2 + 2] cycloaddition cross-linking of the π-stacked layers in 3D COFs. The reaction is reversible, and heating to 200°C leads to a cycloreversion while retaining the COF crystallinity. The resulting difference in connectivity is manifested in the change of mechanical and electronic properties, including exfoliation, blueshifted UV−vis absorption, altered luminescence, modified band structure, and different acid-doping behavior. The Li-impregnated 2D and 3D COFs show a significant room-temperature ion conductivity of 1.8×10^{-4} S/cm and 3.5×10^{-5} S/cm, respectively. Even higher room-temperature proton conductivity of 1.7×10^{-2} S/cm and 2.2×10^{-3} S/cm was found for H_2SO_4-treated 2D and 3D COFs, respectively.

FIGURES



Carbon Nanotube- and Graphene Oxide / 2D Oligoglycine Tectomer Composites and Coatings

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Amino-terminated oligoglycines non-covalently self-assemble, through cooperative hydrogen bonding formation, into biocompatible rigid 2D nanostructures called tectomers, either in solution or in surface-promoted processes [1,2]. Tectomers effectively coat carboxylated multi-walled carbon nanotubes (MWCNT-COOH) and strongly interact with graphene oxide (GO). Electrostatic interactions and hydrogen bonding formation accounts for the strong interfacial interaction of tectomers with MWCNT-COOH and GO, respectively. The resulting composites were characterized by electron- and atomic force microscopies, UV-vis and X-ray photoelectron (XPS) spectroscopies and contact angle measurements [2].

Because of this high affinity of tectomers to GO, tectomers efficiently coat wet-spun GO fibers (Fig. 1). We also show that, due to their versatile surface chemistry, tectomers act as supramolecular peptidic adhesives for the immobilization of a variety of carbon nanomaterials, nanoparticles, molecules and drugs on the GO fiber surface therefore allowing GO fiber functionalization. The resulting ultrathin coatings exhibit remarkable water-resistant properties. This tectomer-based "double-sided sticky tape" fiber functionalization strategy can be extended to other fibers, fabrics and substrates, making it very attractive for technological and smart textile applications [3].

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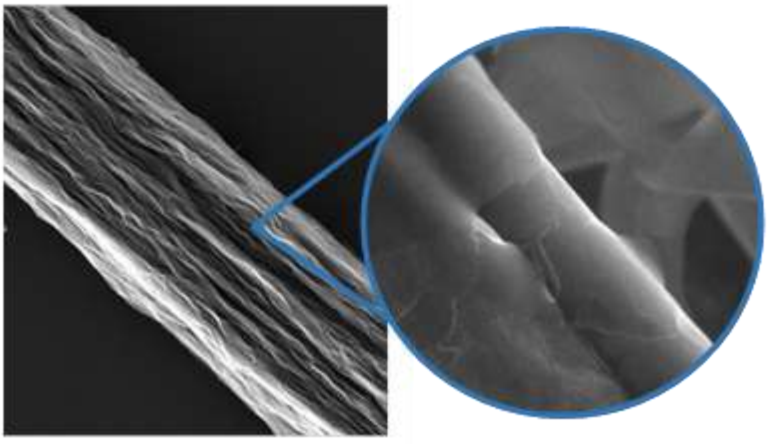

Figure 1: GO fiber coated by ultrathin oligogycine 2D assemblies (tectomers).

Chemical vapour deposition synthesis of MUV-1-Cl magnetic layered coordination polymer and study of the crystal growth process

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The Chemical Vapour Deposition (CVD) technique has been focused by researchers recently as an important tool in the synthesis of layered materials in order to obtain them directly as single or few layered high quality single crystals at large scale and already deposited onto substrates[1]. Using this technique, the aim is the massive production of homogenous 2D molecular magnet crystalline sheets to facilitate their further use in devices and other applications. In this line, coordination polymers have gained the attention of researchers since some of these materials have layered structures[2] and can be obtained in a vapour phase reaction. Furthermore, they are good candidates for applications as, for example, gas sensing or its integration with other 2D materials (for instance 2D superconductors).

Here I will present the development of a CVD synthesis procedure for the synthesis of large thin crystals of a layered iron (II) and 5-chloro-benzimidazolate coordination polymer (MUV-1-Cl). This material has been previously obtained in our group by J. López-Cabrelles in a solvent free reaction under vacuum in a sealed ampoule[3]. The crystals obtained were found to be spin canted antiferromagnets and, interestingly, the surface could be functionalized at will by changing the benzimidazole derivative ligand and, therefore, modifying the surface properties obtaining a whole new family of Layered Coordination Polymers. However, until now, the 2D crystals obtained for this purpose by mechanical exfoliation are not compatible with large scale applications. In order to overcome this limitation, we propose this CVD process in which the production of large and thin 2D crystals (**Figure 1**) has been accomplished and the reaction followed step by step to understand better the growth of these crystals.

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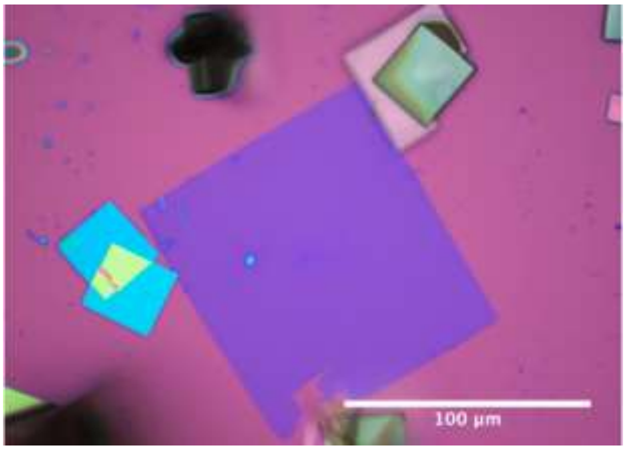

Figure 1: Optical microscope image of a MUV-1-Cl 2D crystal synthesized by CVD.

Unusually Low heat of Adsorption of CO_2 on AlPO and SAPO Molecular Sieves

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Adsorbents combining molecular sieving properties and low heats of adsorption of CO_2 are of clear interest in CO_2 separation processes as they will provide high selectivities and regenerabilities. Materials that have been studied as adsorbents for CO_2 include carbonaceous materials, metal organic frameworks (MOFs), covalent organic frameworks (COFs), supported amines, zeolites, AlPOs and SAPOs [1]. Selectivity, working capacity and easiness of regeneration are the three parameters to be maximized in the selection of an adsorbent. Out of the mentioned materials, supported amines and some MOFs and low silica zeolites interact chemically with CO_2. The CO_2/CH_4 and CO_2/N_2 selectivities on these materials is usually very high, due to the specific interaction between the CO_2 and the adsorbent. However, this strong interaction also leads to large amounts of energy required for regeneration. Adsorption of CO_2 on high and pure silica zeolites, together with carbonaceous materials, many MOFs and AlPOs and SAPOs takes place via a physisoprtion mechanism, which means that the interaction between sorbent and sorbate is weaker, thus meaning regeneration will be less energy intensive. Nevertheless, this does not mean that CO_2/CH_4 and/or CO_2/N_2 selectivities have to be low [2]. In this work, we have studied the adsorption of CO_2 on AlPOs and SAPOs with LTA, CHA and AFI structure and compared the calculated isosteric heats of adsorption with those of analogous zeolites previously reported. The surprisingly low isosteric heats of adsorption (13-25 KJ/mol) found in these materials suggest that AlPOs and SAPOs can present major advantages in the field of CO_2 separation and adsorption in comparison to zeolites, if materials with structures that maximize selectivities of CO_2 over methane or nitrogen are found. This could mean a great improvement in the regeneration process compared to the most frequently used zeolitic adsorbents for this application while maintaining most of their adsorption capacity and selectivity [3].

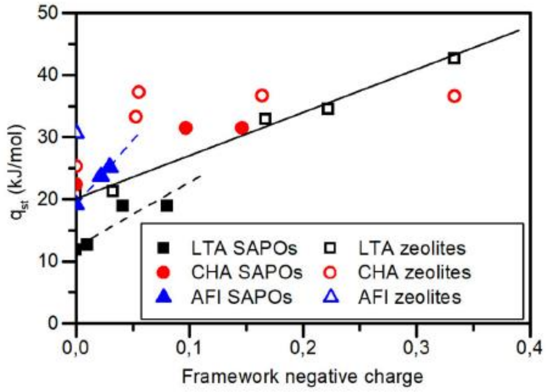

Figure 1: Isosteric heats of adsorption of CO_2 at low loading on zeolites (open symbols), AlPOs and SAPOs (filled symbols)

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Application of Ruthenium complexes in the ammonia electro-oxidation

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For a long time, the scientists are trying to develop water into a cheap, abundant and safe source of hydrogen, thus revolutionising alternative energy field. However, the problems with a high overpotential of the coupled oxygen-evolving reaction (OER), the pH-dependent performance of known catalysts and low stability of catalysts stimulated the development of an alternative approach based on NH_3 splitting. [1]

Ammonia splitting into H_2 and N_2 via ammonia oxidation reaction (AOR), when compared to water splitting, profits from higher thermodynamic favourability and to that related lower energy demands ($E^0 = 0.092$ V vs $E^0 = 1.23$ V vs NHE). [1] Further advantages appear when ammonia is compared directly to hydrogen as an energy carrier, as it is liquefiable at only 8 atm. at room temperature while providing 1.5 more hydrogen density than liquid hydrogen itself. [1]

Looking at the similarities between NH_3 and H_2O chemistry, one can wonder whether OER's catalysts might also be used in AOR. Indeed, recent literature reports provide encouraging reports about the viability of this idea. [2] Herein, we would like to report the results of our study of two different water oxidation catalysts previously developed in our group and recently tested in electrochemical AOR. First, is our original OER RuTda catalyst (Figure 1, left) [3], which mode of action, when compared to literature [4], illustrates the need of the reaching high oxidation numbers at low potentials for good AOR activity. Besides that, we managed to prepare ammonia embedded intermediates and confirm their structure with single-crystal X-ray diffraction. Second discussed family is recently developed oligomeric form of RuBda catalyst (Figure 1, right), which we deposited on the graphitic surface, thus preparing first heterogeneous electrode based on the molecular catalyst for ammonia electro-oxidation. The electrochemical AOR activities of both homogenous (RuTda) and heterogeneous (oligRuBda) systems were then studied under anhydrous conditions as well as in water. Finally, the observed behaviour towards AOR will be discussed in relation to the already known reactivity of these catalysts towards OER.

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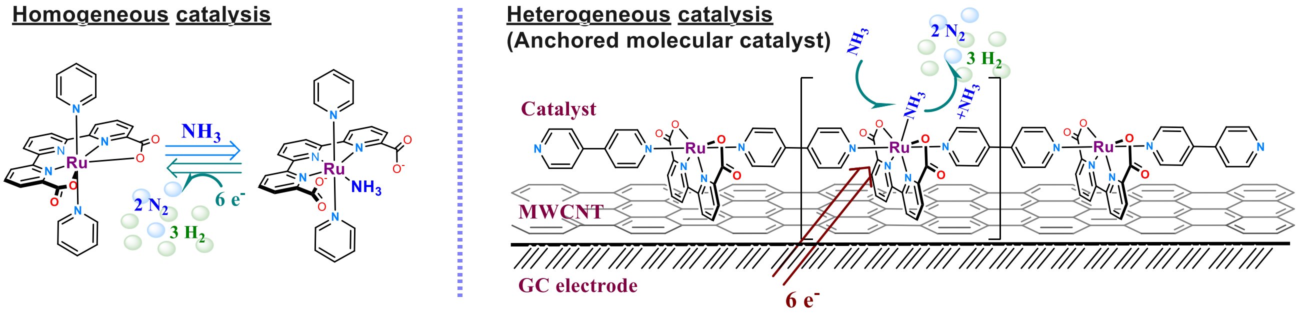

Figure 1: Left: RuTda homogeneously electro-catalysed AOR; Right: Heterogenised oligomeric RuBda AOR catalyst

Sensing switchable molecular systems with 2D materials

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Abstract

Graphene is one of the most studied materials due to its unique properties such as hardness, flexibility and high electric and thermal conductivity. [1] Probably, the best quality of graphene is that it has opened the field to many other 2D crystals [2] and, in particular, to molecular materials.

However, in the field of two-dimensional materials, molecular compounds are still scarce if compare with its inorganic counterparts and even more elusive are magnetic 2D molecular compounds. [3] Although less studied in the 2D-land, molecular systems exhibit new physical phenomenology like the so-called spin-crossover (SCO) transition. SCO materials are metal complexes where the spin state of the metallic center changes between high-spin (HS) and low-spin (LS) due to the presence of an external stimulus (light, pressure, temperature…), with potential applications as memory devices or in spintronic applications [4].

In this work, we fabricate hybrid molecular/inorganic van der Waals heterostructures based on molecular spin-crossover (SCO) materials and inorganic two-dimensional crystals (Figure 1). First, we exfoliate mechanically a SCO compound and characterize it by atomic force microscopy, optical microscopy and Raman spectroscopy. Then, these molecular flakes are deterministically combined with inorganic 2D systems like few-layers graphene (FLG) or atomically-thin layers of 2H-$NbSe_2$ and WSe_2, thus creating hybrid molecular/inorganic van der Waals heterostructures. Interestingly, the hysteretic thermal spin transition is detected by transport measurements in our hybrid van der Waals heterostructures.

Our results illustrate the synergy between SCO and inorganic 2D crystals and opens the door to explore further molecular compounds of interest which properties could not be detected otherwise.

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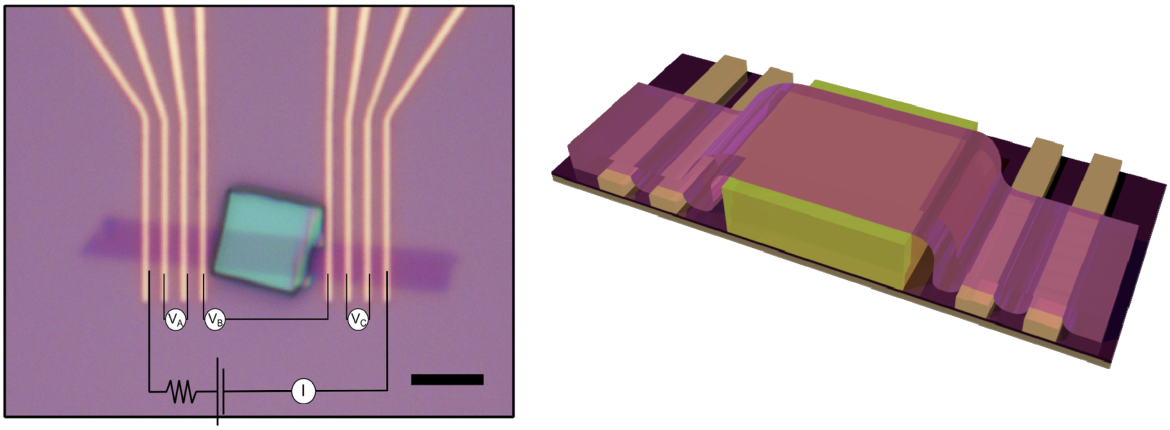

Figure 1: hybrid van der Waals heterostructure based on few-layers graphene and SCO crystals. Left: Device with the electronic transport configuration. Right: Artistic representation where the few-layers graphene is represented in purple, the SCO in yellow and the metal contacts in gold.

Functionalization of Silver Nanowire Transparent Electrodes with Two-Dimensional Oligoglycine Tectomers

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Silver nanowire (AgNWs) networks combine high optical transmission with low sheet resistance that, together with their decreasing cost and large-scale manufacturing methods, make them perfect candidates as replacement materials of Indium Tin Oxide (ITO) for transparent electrode applications, as well as for platforms with potential applications in bio-sensors and bio-engineering [1]. On the other hand, amine-terminated oligoglycines self-assemble into unique two-dimensional nanostructures called tectomers. The exceptional structural features and surface chemistry of tectomers have already been successfully used to coat negatively-charged surfaces, and biological membranes, and have promising potential in the field of antiviral application [2]. Previously we reported that tectomers efficiently act as pH-responsive nanocarriers [3], and showed, for the first time, that tectomers strongly interact with graphene oxide and carboxylated carbon nanotubes [4], and with a variety of other carbon nanomaterials and functionalized nanoparticles [5], offering promise for a range of technological applications and in electronic- and smart textiles [4,5].

We here report on the fabrication of AgNW/tectomer peptidic nanohybrids by coating transparent AgNW electrodes with thin tectomer films. Tectomer platelets strongly interact with AgNWs using the interactions between amino groups and silver atoms, and mechanically compress AgNW networks, leading to the formation of transparent hybrid electrodes with remarkably enhanced electrical conductivity. Tectomer coatings impart moisture protection to AgNW electrodes, preventing electrode degradation upon exposure to atmospheric conditions [5]. The hybridization of AgNW with these unique peptide assemblies creates tremendous opportunities in extending the applications of transparent electrodes in new directions, ranging from sensing to nanoscale electronics to hybrid functional materials [6].

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Preparation of Continuous Highly Hydrophobic Pure Silica ITQ-29 Zeolite Layers on Alumina Supports

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Hydrophobic membranes have been attracted much attention for the separation of molecules based in their polarity and highly hydrophobic pure silica ITQ-29 zeolite may result in a good candidate to carry out such separations. Continuous layers of intergrown ITQ-29 zeolite crystals were successfully grown on porous alumina supports by optimization of the synthesis conditions, such as the appropriate selection of the seeds, the procedure for the gel preparation, and the calcination conditions. This resulted in the formation of all silica ITQ-29 zeolite layers without the presence of germanium required in previously reportedITQ-29 membranes [1], with the subsequent improvement in quality and stability, as verified by the absence of cracks after calcination. We have proved that the incorporation of aluminum from the support into the zeolite layer does not occur, neither during the secondary growth nor through migration of aluminium species during calcination.

The water content of the synthesis gel was adjusted after the silica precipitation, hence resulting in a viscous gel rather than a solid material, thus favouring a better contact with the seeded support. In this way, continuous layers of 8 µm thickness were prepared after 7 days of secondary growth, and were activated by calcination at 773 K in air, resulting in crack-free microporous membranes.

The incorporation of aluminum from the support into the zeolite layer did not occur, neither during the secondary growth nor through migration of aluminum species during calcination. The materials obtained were defect-free and crystalline, being appropriate candidates for bioalcohols [2] separation in aqueous solutions.

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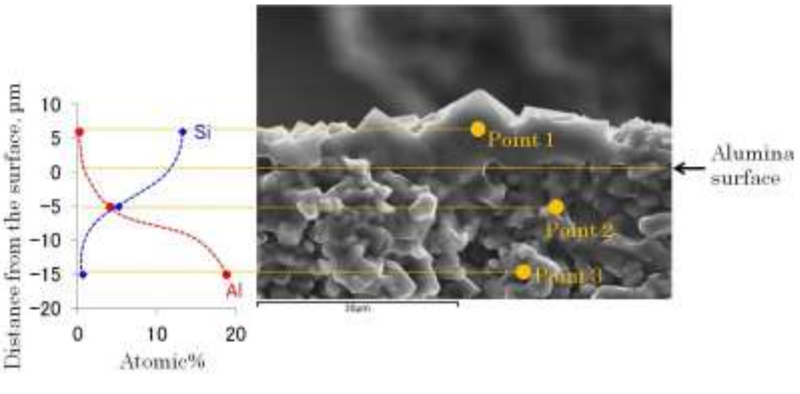

Figure 1: Si and Al composition along the ITQ-29 material grown on the alumina support.

Adsorption of linear, monobranched and dibranched alkanes on pure silica STW zeolite as a promising material for their separation

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Gasoline is a liquid mixture mainly consisting of hydrocarbons in the C4−C12 fractions and is one of the most used fuels worldwide. Its performance is evaluated in terms of the octane number (ON). Hydroisomerization of linear short chain paraffins is an effective method of obtaining higher-octane components for the gasoline blend, i.e. multibranched products. The linear components are separated from the effluent and recycled by means of an adsorption process that uses zeolite 5A as the adsorbent.[1] The ideal target, however, is the separation and recycling of both linear and monobranched hydrocarbons, as the latter ones also present low ON. Medium pore materials with several structures and compositions have been proposed for this separation, out of which silicalite-1 (Si-MFI) is most frequently addressed.[2] Here, we present pure silica STW zeolite (Si-STW) as a material which is superior to Si-MFI for the said separation. The adsorption of linear, monobranched and dibranched saturated hydrocarbons in the gasoline range has been studied on Si-STW by using pentane, hexane, and heptane isomers as model adsorbates. Significant differences in both the equilibrium adsorption and especially the adsorption kinetics were found. The diffusivity increases in the order dibranched quaternary <<< dibranched-α < dibranched-β < monobranched ≈ linear. Size exclusion of quaternary carbon dibranched isomers is demonstrated, with monobranched and linear isomers being preferentially adsorbed on this material. The adsorption capacities and selectivities surpass those of pure silica MFI (Si-MFI) in a factor of ca. 1.5. Altogether, Si-STW is presented as a promising adsorbent for increasing the octane number (ON) of the hydroisomerization product by selectively excluding quaternary carbon dibranched hydrocarbons.

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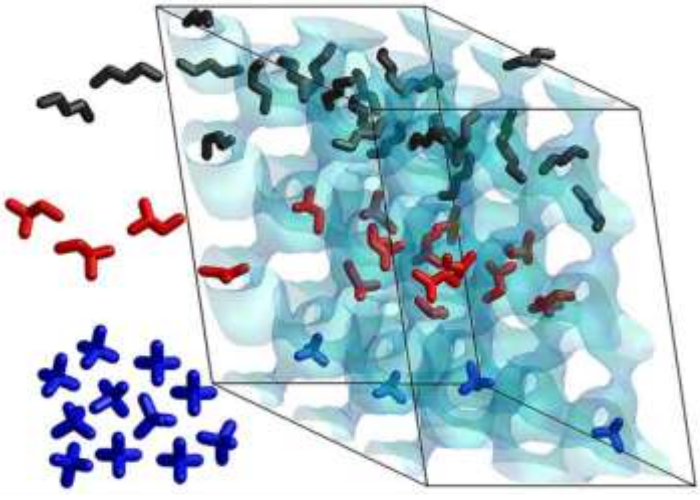

Figure 1: Schematic representation of the adsorptive separation of C5 isomers on Si-STW.

Design of magneto-plasmonic heterostructures formed by Au decorated on magnetic Prussian Blue-type nanocrystals

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Magneto-plasmonic nanoparticles (NPs) (*i.e*. NPs simultaneously showing magnetic and plasmonic properties) have become in recent years an active topic of research. These materials find applications, for example, in nanophotonics, optical biochemosensing or storage data [1]. In general, magnetoplasmonic particles are formed by the combination of noble and ferromagnetic metals. Thereby, magneto-optical activity of these hybrid systems can be greatly increased due to the plasmon resonance effect provided by noble metal nanoparticles [2]. The study of new magnetoplasmonic systems with an efficient coupling between magnetic and plasmonic properties is a burgeoning research field. In this context, some Prussian Blue Analogues (PBAs) have been proven to be excellent candidates for magneto-optical applications [3] due to their transparency in the visible region and their several advantages with respect to other conventional inorganic materials [4].

Here, we have developed a general protocol for the preparation of hybrid nanostructures formed by NPs of molecule-based magnets based on PBAs decorated with plasmonic Au NPs of different shapes (see Figure 1). By adjusting the pH, Au NPs can be attached preferentially along the edges of the PBA or randomly on the surface. The protocol allows tuning the plasmonic properties of the hybrids in the whole visible spectrum.

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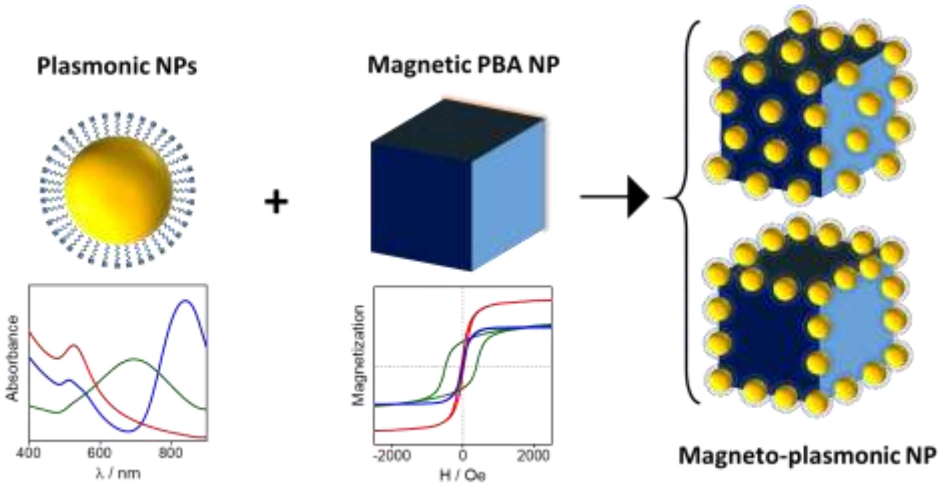

Figure 1: Scheme of the magneto-plasmonic heterostructures formed by the decoration of Au on PBA NPs.

Covalent functionalization of non-aluminium layered double hydroxide with tripodal ligands.

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Layered double hydroxides (LDHs) are a class of cationic layers with exchangeable anions in the interlayer space that exhibit a hydrotalcite-like structure. The high tunability regarding metallic composition, stoichiometry, and the interlayer anion gives LDHs a wide versatility; resulting in different applications such as catalysis, sensing, magnetism or energy storage, to name a few.[1] Furthermore, the anionic behaviour of these 2D materials allows the design of several hybrid heterostructures through electrostatic interactions.[2,3] In this field, a further step would be the covalent functionalization of LDH, allowing these attractive materials to be endowed with new properties and creating more complex hybrid heterostructures. With this goal in mind, the covalent functionalization of LDHs is being investigated by our group, indeed we developed a pH-reversible covalent functionalization with aminopropyl triethoxysilanes (APTES) of the NiFe–LDH.[4] However, in view of the poor stability at basic pH (typical pH for electrochemical applications) of this covalent bond, we have performed a new stable functionalization at basic pH with tris(hydroxymethyl) aminomethane (Figure 1) of LDHs with different compositions (NiFe, CoFe and NiV-LDHs), using an modified hydrothermal method from Kuroda et al.,[5]. This new family of LDHs has been studied by means of X-ray diffraction, infrared spectroscopy, thermogravimetric analysis coupled with mass spectrometry, X-ray photoelectron spectroscopy, transmission electron microscopy and energy-dispersive X-ray spectroscopy, among others. In addition, its magnetic and electrochemical behaviour was explored. Reactivity studies have been carried out on the terminal amino group, as well as protonation and deprotonation, to modify the behaviour in terms of the polarity of these materials. This new level of manipulation in LDHs can be used to design novel heterostructures on-demand and improve the exfoliation of these appeling materials.

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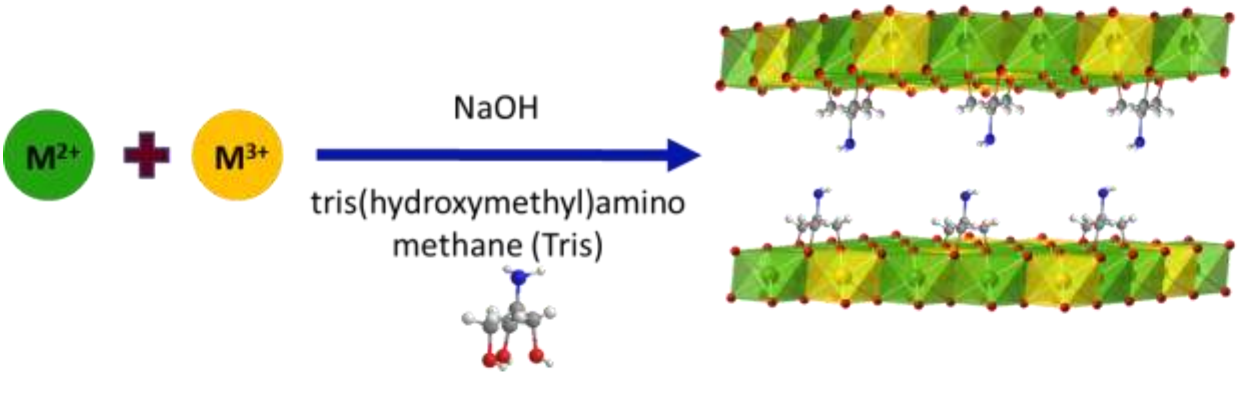

Figure 1: Synthesis of covalently functionalized LDHs with tripodal ligands.

Smart molecular/MoS_2 Heterostructures to Thermally-Induced Strain Driven by Spin Switching

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Layered two-dimensional transition-metal dichalcogenides (TMDCs) have garnered intense attention due to the different properties achieved by modifying their composition and number of layers. One of the most studied members of this family is the MoS_2. This compound is an indirect bandgap semiconductor that turns to direct-gap when is exfoliated from bulk down to a monolayer, which makes it very promising for its integration in electronic, optoelectronic, and photovoltaic devices.[1] Recently, many studies have focused on altering its electrical and optical response via strain engineering.[2]

In this work, we propose an original approach to induce a reversible strain on MoS_2 ultrathin layers. It consists of the 2D surface functionalization with switchable molecular systems that undergo a reversible volume change upon applying an external stimulus. In this context, we propose using spin-crossover (SCO) nanoparticles as mechanical actuators. These SCO materials can change their ground spin state between low spin (LS) and high spin (HS) upon the exertion of various external physical or chemical stimuli, resulting in a variation in the nanoparticles volume depending on the spin state.

In this context, we have achieved the decoration of MoS_2 flakes with SCO nanoparticles (Figure 1a) of the well-known SCO compound $[Fe(Htrz)_2(trz)](BF_4)@SiO_2$.[3] This material presents a transition above room temperature with a broad hysteresis, 40 K, and a change in volume of ca. 10 %. The hybrid composite exhibits an abrupt change in conductivity near the NPs transition temperature (Figure 1b), which can be associated with a decrease in the bandgap. Even more, the narrowing of the bandgap, caused by the spin transition, is monitored by following the composite photoluminescence in both spin states. Corroborating the conductivity results, the expected energy shift of the MoS_2 bandgap is detected after the spin transition (Figure 1c).

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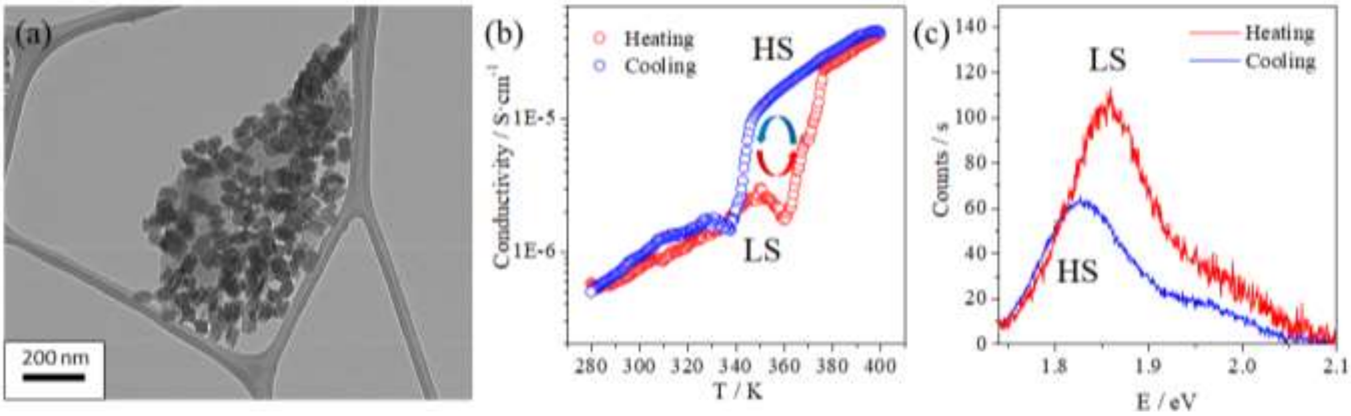

Figure 1: (a) HR-TEM images of the decorated MoS_2. (b) thermal variation of the conductivity in the heating and cooling modes of the heterostructure. (c) PL spectra of the same composite in LS and HS state.

ePOSTERS

Formation of Archimedean Tessellation Found in the Mixtures of Pentatopic and Linear Molecules

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Abstract

Supramolecular chemistry is of particular interest for past few decades. Many either theoretical or experimental papers have been published about various classes of molecules, which are able to self-assembly on solid surfaces [1, 2]. Particularly interesting are rigid organic compounds of diverse architectures that tend to form different molecular networks by means of directional bonding between “active” groups. Such interactions may be, for instance hydrogen bonding and in the case, when the metal atoms are present - donor-acceptor interactions, which lead to coordinate bonding between metal and active groups. Hence, ability to self-assembly could be used in material chemistry and especially for producing new class of the so called "smart materials". Their application is mainly focused in fields like photonics, electronics, drug delivery systems and so on.

In this work, we present the results of molecular dynamics simulations for two cases, (i) single-component systems involving the tetra-, penta- and hexatopic [3, 4] molecules and (ii) for their mixtures with linear and V-shape particles. For the latter case, we have changed the chemical composition of the mixture and checked its influence on the formed ordered structures. We have found that, in the mixture of a pentavalent molecule and linear linker, the Archimedean tiling has been formed, which has not been the case in the single-component system. We have concluded that, for this case, the mobility of the linker is the driving force.

All of the formed structures have been further characterized by several quantities such as bond order parameter and other distribution functions.

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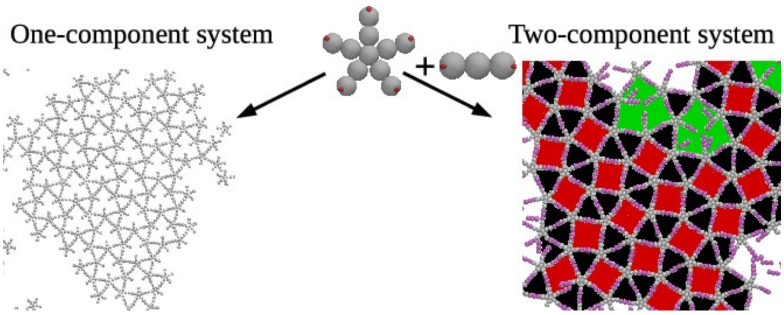

Figure 1: Presentation of different networks fromed by pentatopic molecule either in one-component system or two-component system with linear linker.

Enhancement of a hollow fiber filter via a graphene oxide coating

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Abstract

In the recent years, new classes of contaminants are consistently being found in the ground and even in drinking water supplies. The occurrence of these compounds, known as emerging contaminants (ECs), in water supplies may lead to severe environmental pollution and health problems [1]. Several studies suggest that the use of membranes doped with nanomaterials represent a promising strategy to address this crucial issue. Among nanomaterials, graphene oxide (GO) is considered one of the most suitable choices for this use, due to its unique chemophysical properties, versatile potential for covalent functionalisation and commercial availability in large amount and good standard quality [2]. Polyethersulfone-polyvinylpirrolidinone hollow fibers (PES) are commercially available microfiltration membranes used as active components of modules for blood filtration and water disinfection. PES microfiltration mechanism relies majorly on size exclusion, thus making these filters ineffective for the removal of small molecules such as drugs. However, PES hollow fibers are suitable for surface modification with GO, allowing the production of PES-GO core-shell hollow fibers and derived filters, which combine the microfiltration mechanism of PES with the adsorption capability of GO [3]. This composite material allows a synergic and efficient removal of both nanoparticles, through microfiltration, and small molecules, through adsorption by intercalation between GO layers, as demonstrated by combined X-Ray Diffraction experiments and molecular modelling. In this communication, we describe the fabrication of core shell PES-GO hollow fiber filters and their use for simultaneous removal of several contaminants.

Figure 1: Core-shell hollow fiber PES-GO cartridge for synergic microfiltration and adsorption of microcontaminants from drinking water.

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Salting out and interfacial tension of methane with electrolyte solutions from computer simulations

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The solubility of methane in water decreases when a small amount of salt is present. This is usually denoted as the salting out effect (i.e., the methane is expelled from the solution when it contains small amounts of salt). The effect is important, for instance the solubility is reduced by a factor of three in a 4 m (mol/kg) NaCl solution. Some years ago, we showed that the salting out effect of methane in water could be described qualitatively by molecular models using computer simulations [1]. However, the salting out effect was overestimated. In fact, it was found that the solubility of methane was reduced by a factor of eight. This points out to limitations of the force field used. In this work [2] we have carried out direct coexistence simulations to describe the salting out effect of methane in water using a recently proposed force field denoted as Madrid-2019 [3] based on the use of scaled charges for the ions and the TIP4P/2005 force field for water [4]. For NaCl the results of the Madrid-2019 force field significantly improve the description of the salting out of methane as can be seen in Fig. 1. For other salts the results are quite reasonable. Thus, the reduction of charge of the ions seems also to be able to improve the description of the salting out effect of methane in water.

Besides, we shall show that the brine-methane interface exhibits an increased interfacial tension as compared to that of the water-methane system. It is well known that electrolytes tend to increase the surface tension of liquid water, and this seems also to be the case for the interface between water and methane.

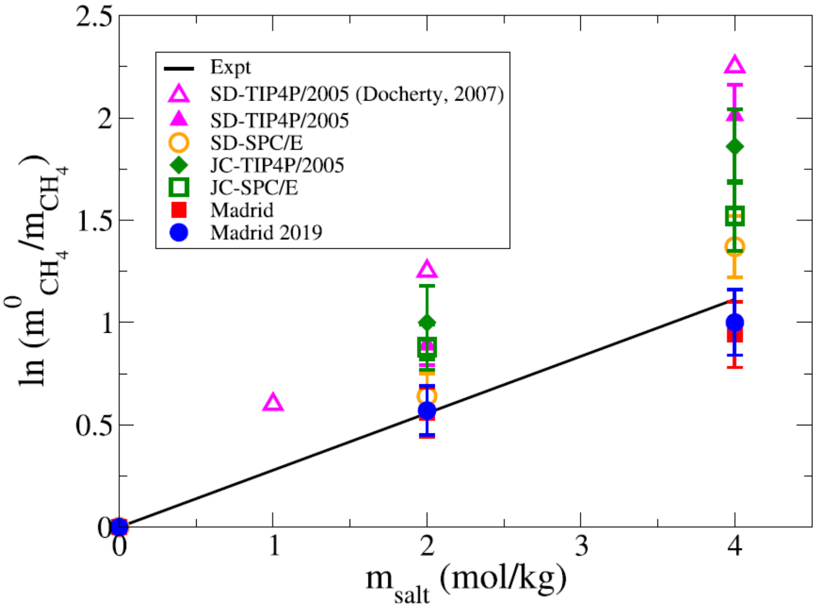

Figure 1: Salting out of methane calculated from computer simulations with different models

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Selective Discrimination of Toxic Polycyclic Aromatic Hydrocarbons in Water by Targeting π-Stacking Interactions

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The development of highly sensitive and selective devices for rapid screening of polycyclic aromatic hydrocarbons (PAHs) in water is nowadays a crucial challenge owing to their alarming abundance in the environment and adverse health effects. Herein, inspired by the unique π-stacking interactions taking place between identical small aromatic molecules, a novel, generic, and straightforward methodology to electrochemically determine and discriminate such pollutants is described. Such a method is focused on covalently anchoring different PAHs on an indium tin oxide electrode surface by means of self-assembled monolayers. The surface-anchored PAHs act as recognition units to selectively interact with a specific PAH target of the same nature. By tailoring the recognition platform with four different models PAH molecules (naphthalene, anthracene, pyrene, and fluoranthene) and carrying out an electronic tongue approximation, the selective discrimination and quantification of the selected PAHs in aqueous samples at ultralow concentrations were achieved impedimetrically, which were also validated using a certified reference PAH mixture. [1-2]

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FIGURES

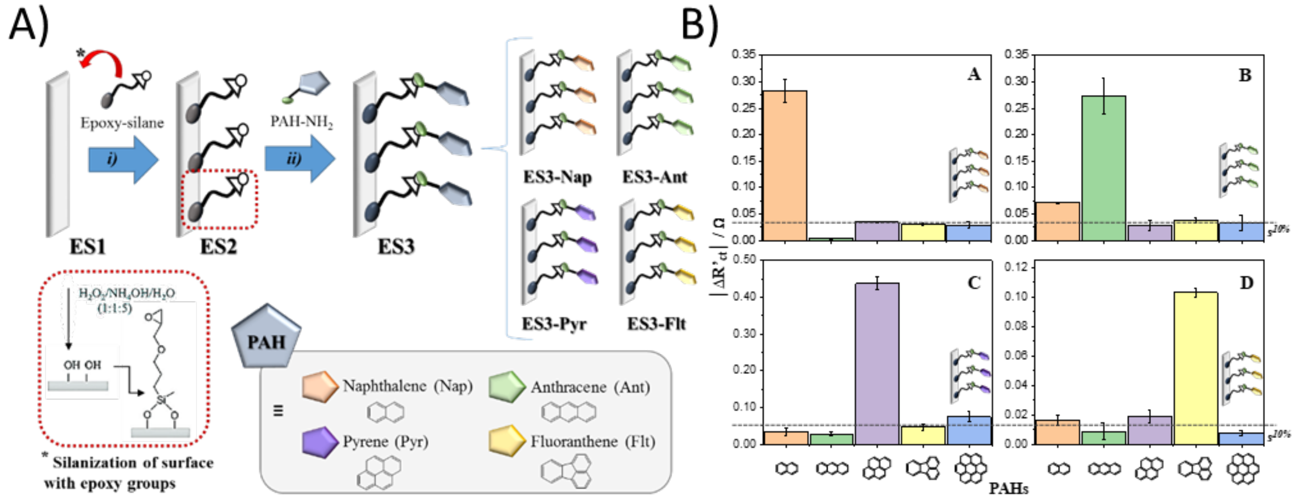

Figure 1: A) Schematic Representation of the Four PAH-Based Recognition Platforms Synthesized on ITO Electrodes (ES1); (i)Electrode Activation in an Oxidation Bath and Epoxy-Silane SAM Formation (ES2); (ii) Covalent Grafting of the PAH−NH2Recognition Units via Epoxy-Amine Cross-Linking (ES3). **B)** Electrochemical anti-interfering assay at the (A) ES3-Nap, (B) ES3-Ant, (C) ES3-Pyr, and (D) ES3-Flt using five different PAH analytes (Nap, Ant, Pyr, Flt, and Cor) with a 2 ppt concentration.

Interaction between hexon protein from Adv 5 and pegylated-icosahedral gold nanoparticles

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Understanding the interaction of proteins with gold nanoparticles is vital to the development of new detection methods, delivery drugs or vaccines. In particular, the control over the type of interaction (covalent or non-covalent) between gold nanoparticles (AuNPs) and proteins present in viruses can represent a great advance in this context. For this reason, this work evaluates the effectiveness of attachment of hexon protein from Adv 5 at icosahedral AuNPs. For this purpose, a new protocol for the modification of icosahedral AuNPs (which are covered with CTAB from the synthesis) with PEGs has been developed, obtaining totally stable pegylated-AuNPs. As it can be seen in the Figure 1, the icosahedral AuNPs were coated with different types of polyethylene glycols (PEGs) such as methoxy-PEG-thiol (mPEG-SH) and thiol-PEG-amine (SH-PEG-NH_2). When mPEG-SH was used, hexon protein interacted with AuNPs through hydrophobic and therefore reversible forces. On the contrary, when icosahedral AuNPs were modified with SH-PEG-NH_2 and subsequently with glutaraldehyde, imine groups were formed between the NH_2 residues of the Hexon protein and the glutaraldehyde. The resulting NPs were characterized by TEM, UV-vis, DLS, IR, and XPS.

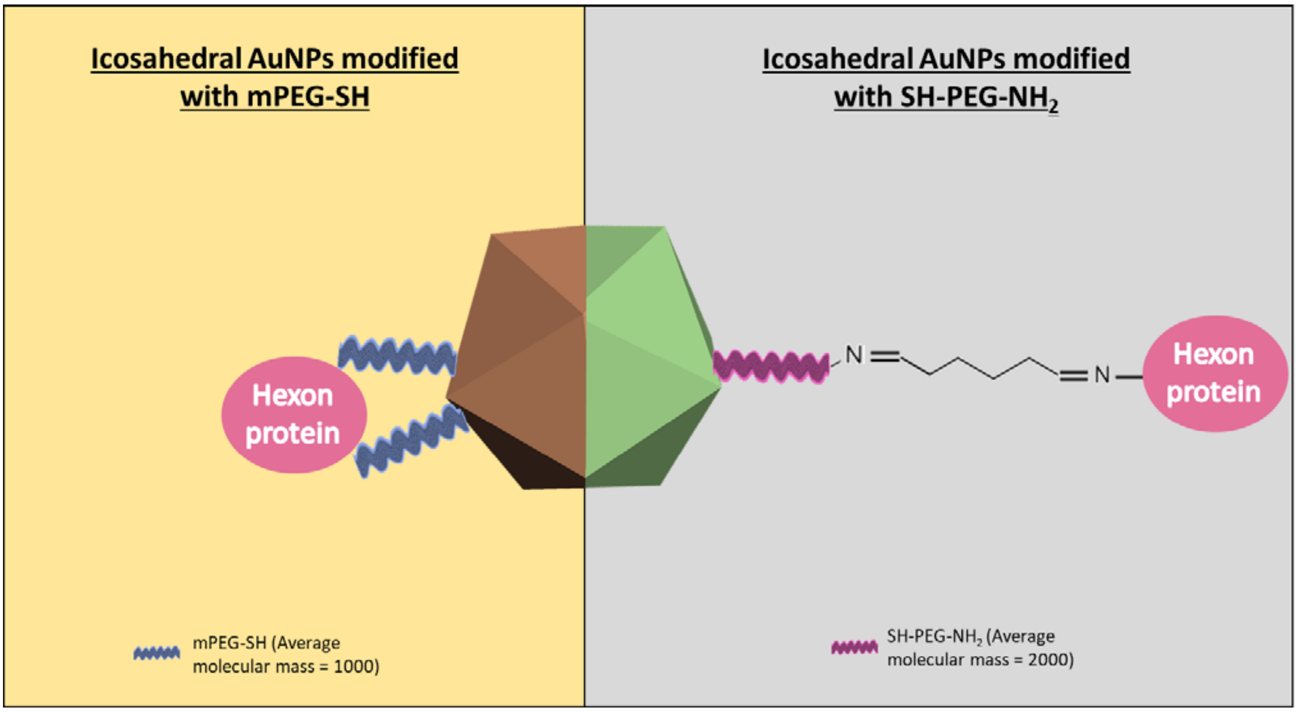

Figure 1: Covalent and non-covalent attachment of hexon protein to pegylated icosahedral AuNPs.

Polyoxometale-Stabilized Metal Nanoparticles: Potential Candidates for Energy Storage Applications.

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ABSTRACT: Polyoxometalates (POMs), redox active anionic metal–oxide clusters, display an extraordinary range of physicochemical properties and are some of the most promising building blocks for functional nanomaterials. The most important functionality of POMs involves their unique electrochemical behaviour.[1] Due to the high stability of their redox states, they can participate in fast reversible multielectron-transfer reactions, making them potential candidates to achieve a high capacity for energy storage applications. Anchoring POMs on carbon materials effectively increases the number of electroactive sites for electrochemical reactions. Indeed, POM−based hybrid electrodes with a variety of nanocarbon materials have been reported.[2-5] This combination is particularly effective for applications in hybrid supercapacitors (SCs) that combine the high power and long-term stability of SCs and the high energy density of batteries, as the carbon support contributes double-layer capacitive effects, while the POM provides faradaic charge storage.[6] However, POMs have poor electrical conductivity, which can have a detrimental influence on specific capacitance and cycling stability.

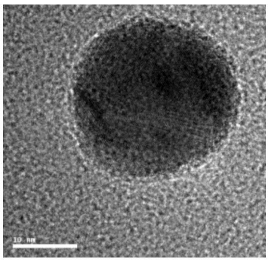

***Figure 1**. TEM image of POM-stabilized Silver NPs.*

Nobel metal (M^0) nanoparticles (NPs) have been widely used as conductive dopants in electrode materials for SCs due to their good conductivity and electrochemical stability.[7,8] By combining POMs with M^0 NPs, it is hoped to promote desirable synergistic properties and functionalities and yield composites with improved capacitive performance and cycle life. Moreover, the combination of M^0 NPs with carbon materials enhances the electrical double layer capacitance by providing larger electrochemically active materials.[9] POMs have been exploited for directing the synthesis of M^0 NPs.[10] POM−stabilized M^0 NPs have received enormous attention because of their unique chemical and physical properties with different applications (catalysis, biosensors, biomedicine).[11] However, their use in electrochemical energy storage remains largely unexplored. Hence, this work presents an optimized green and reproducible protocol of synthesis to obtain M^0 NPs stabilized with POMs, with low polydispersity and high stability. Their morphological properties are characterized using electron microscopy (**Figure 1**) and their structural and chemical properties are analysed using X-ray diffraction, X-ray photoelectron spectroscopy, IR spectroscopy and electrochemical methods. Finally, we present the incorporation of the M^0 NPs with POMs and activated carbon to create a hybrid tri-component composite electrode. The composite is characterized and its potential as electrode material for energy storage application is preliminary assessed.

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Graphene-polysulfone sorbents for the removal of contaminants of emerging concern from drinking water

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The recently adopted European Drinking Water Directive EU 2020/2184 impose the monitoring and removal of new contaminants such as per- and polyfluoroalkyl substances (PFAS) from our drinking water and tighten the limits for already regulated substances. Such stringent requirements are pushing academic and industrial research to the development on new materials and strategies for efficient water treatment. Graphene based materials, due to their high surface area and multiple interactions pathways with organic molecules and metal ions allowed by the abundant surface chemical moieties, have shown great potential for water purification purposes [1]. Here, we present the preparation of a graphene oxide-polysulfone-composite (PSU-GO) [2] and its use as sorbent for the removal of contaminants of emerging concern from drinking water, including PFAS and lead. Polysulfone granules were obtained by processing of scraps of industrial production of hollow fiber membranes (Medica spa). PSU-GO (2.5% w/w in GO) was prepared by using a water based and microwave assisted process, requiring mild conditions. [3] The so obtained filters showed high versatility since they removed lead ions, antibiotics and a selection of PFAS of current concern from tap water. The performance and working mechanism of the new composite will be described.

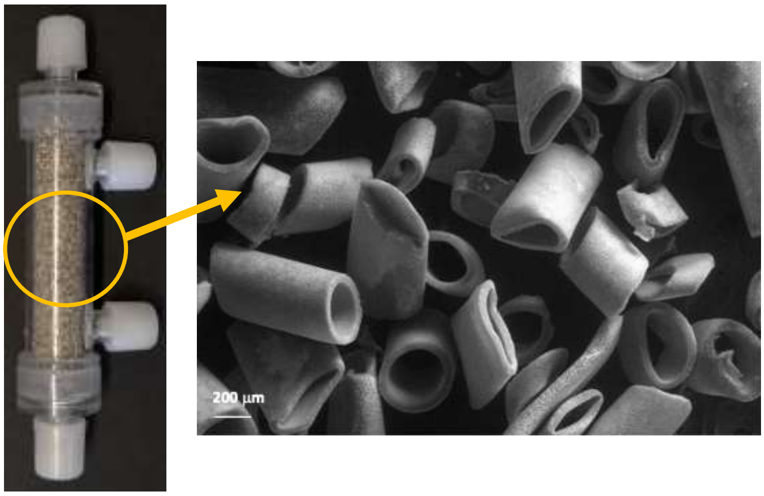

Figure 1: Image of PSU-GO cartridge and granules

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Customizable SERS substrates dedicated for life science and diagnostic research

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Surface-Enhanced Raman Spectroscopy (SERS) is gaining popularity in the field of life science as it allows us to obtain the fingerprint of a specific substance or even cell type. Thus, SERS is now intensively studied as a promising tool for diagnostic [1], [2] and pathogen identification. SERS-based biosensors and microfluidic systems may be fast and accurate platforms for detecting cancer, food contamination [3], and even viruses identification.

We recently developed sensitive and repeatable SERS silver and silver-gold substrates dedicated for potential use in biosensors and microfluidic systems in diagnostic and life science research. Our platforms are made by the electrodeposition of silver and gold nanoparticles on ITO glass. Our substrates have dimensions dedicated to 96-well plates and give great enhancement in SERS measurements after compound deposition in a small volume and a low concentration (ppm to ppb) of an analyzed solution. Additionally, thanks to a precise laser plotter, we can obtain defined dimensions of substrates. It is especially desirable for the development of “Lab-on-a-Chip” type platforms. Our substrates can exhibit different surface properties on custom demand - hydrophilic or hydrophobic. Hydrophilic substrates give excellent enhancement of aqueous solutions, whereas hydrophobic are dedicated to alcoholic solutions.

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FIGURES

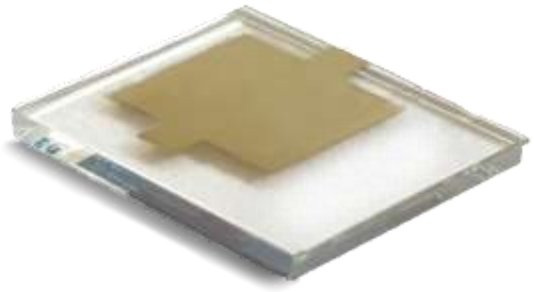

Figure 1: Customizable SERS substrate with nanoparticles surface on ITO glass.

Synthesis and high-performance purification of functionalized graphene for water treatment

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Covalent modification of graphene oxide is a widely exploited strategy to tailor the surface and structure of graphene and enable new applications [1]. Several functionalized graphenes have been reported for water purification applications. Among them, covalent binding of branched polyethilenenimine (PEI) has revealed great potential for the removal of metal ions from water [2] and for realizing membranes for ion sieving [3] Here we report an unprecedent strategy allowing fast and efficient synthesis and purification of GOPEI. Microwave assisted epoxide ring opening combined to microfiltration on commercial hollow fiber modules allows to achieve GOPEI (63% yield) in only 30 minutes of MW irradiation at 80°C. PEI loading of about 40% was easy estimated by taking advantage of the microfiltration cartridge working mechanism (Fig. 1). The so obtained GOPEI nanosheets were exploited for arsenic and lead removal from water and the performances related to the surface properties (i.e. charge, polarity and structure) of the functionalized graphene.

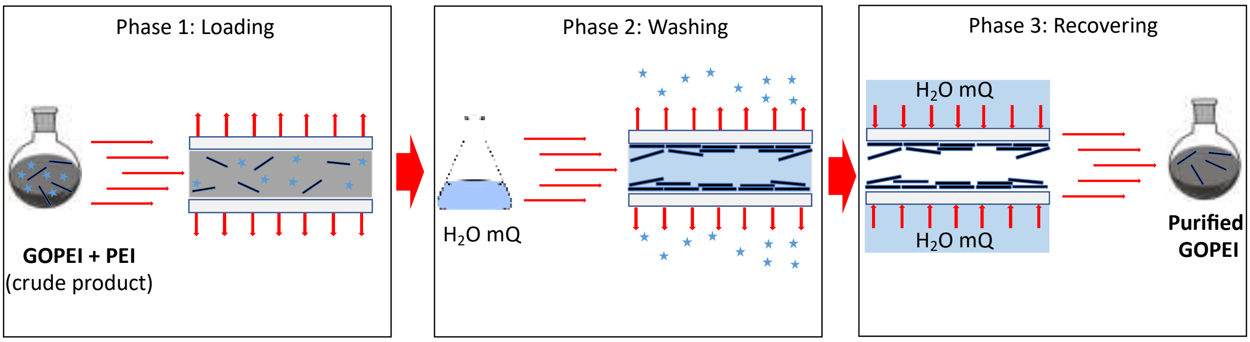

Figure 1: Sketch of the microfiltration procedure developed for modified GO purification. The crude material is introduced in the filtration module, the sheets are stopped by the membrane pores (cut off 100 nm) and washed and finally detached by inverting the water flow direction.

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Chromogenic chemodosimeter based on capped silica nanoparticles to detect spermine and spermidine.

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High levels of polyamines such as spermine (Spm) and spermidine (Spd) have proven to be interesting biomarkers in the detection of diverse pathological situations[1-3]. Therefore, the design and synthesis of new probes is a field of research in constant development and of great interest[4-5] since they can be used to detect the presence of these polyamines in biological fluids and tissues with no need of expensive instruments.

Hence, a new material based on MCM-41 functionalized with a N-hydroxysuccinimide derivative and loaded with rhodamine 6G has been developed for the sensing of Spm and Spd. The dye is kept inside the porous due to a double layer formation of organic matter. The inner layer is covalently bound to the silica nanoparticles and the external one is formed through hydrogen and hydrophobic interactions. Removal of the external coverage, in amine groups presence, opens the pores allowing the dye to release. The release studies were performed through fluorimetric titrations, obtaining limits of detection of 2.7x10-5 M for Spm and 4.5x10-5 M for Spd. The sensor remains silent in the presence of other biologically important amines and can detect Spm and Spd in aqueous solution and in cells.

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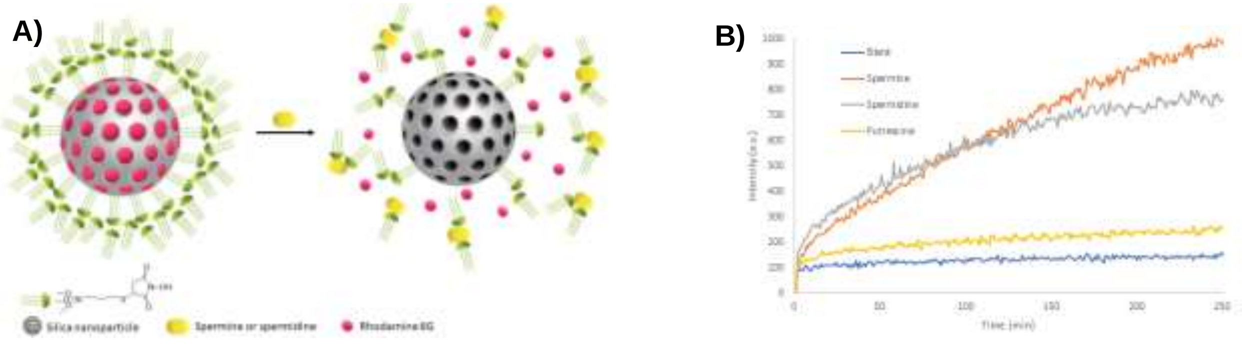

Figure 1: A) Sensing protocol for detecting Spm and Spd. **B)** Rhodamine 6G delivery profiles from the material in the absence and presence of Spm, Spd and putrescine.

Functionalized gold nanoparticles to detect GHB in aqueous media

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One of the most substantial problems present in our society is the consumption and abuse of drugs. Specifically, the practice of sexual crimes associated with drug use, called Drug-Facilitated Sexual Assault (DFSA) is a big concern. Many different compounds used in DFSA assaults have been identified, but among them γ-hydroxybutyric acid (GHB) is one of the most elusive.[1] Even though GHB presents suitable characteristics to be employed in medicine; it has also been used as an illicit drug because of its euphoriant and aphrodisiac properties. There are two reasons for its use as a rape drug: first, a high dose intake promotes a loss of conscious and second, it is difficult its detection due to its organoleptic properties.[2]

For this reason, we have developed a real time detection probe based on doubly functionalised gold nanoparticles (AuNPs). These AuNPs have been functionalized with a napthoxazole moiety, to recognise the carboxylic group,[3] and a phenanthroline derivate, to interact with the alcohol.[4] Once the double recognition takes place, AuNPs aggregate and a remarkable colour change is observed due to the plasmon band shift, from red to blue.

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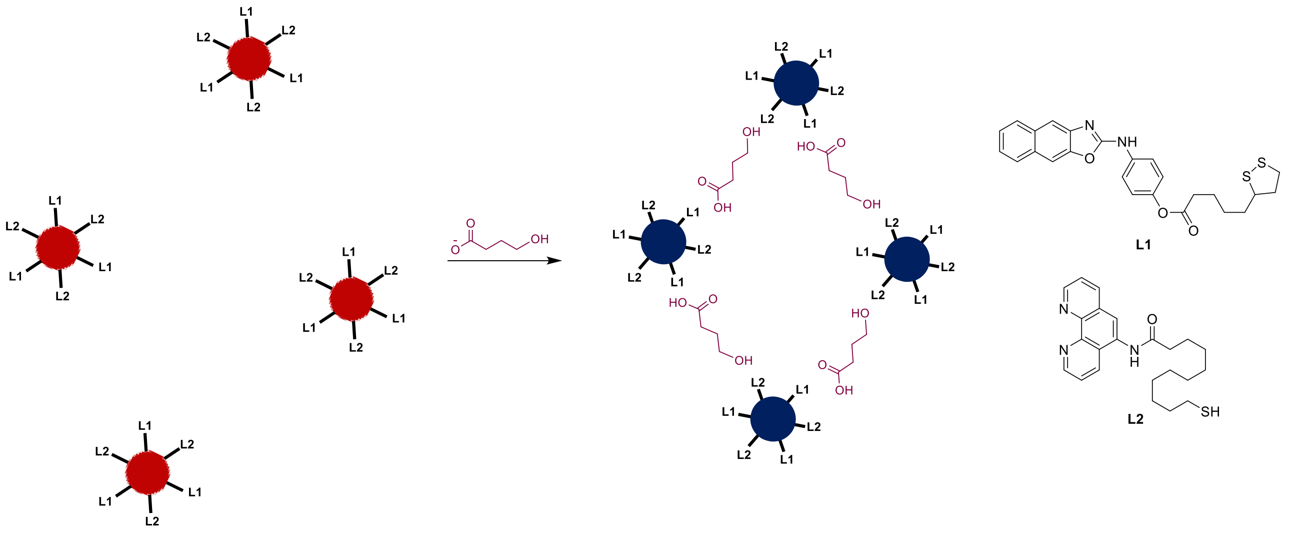

Figure 1: Recognition paradigm based on AuNPs functionalised with **L1** and **L2**

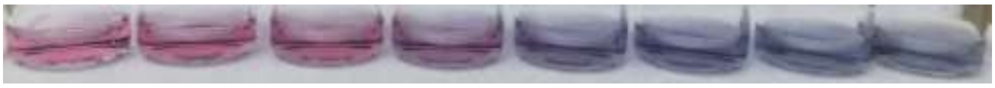

Figure 2: Colour changes observed due to the GHB recognition

Protection against chemical submission: naked-eye detection of ϒ-hydroxybutiric acid in soft drinks and alcoholic beverages

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Chemical submission in an important social problem associated with sexual aggression. Among the compounds used by criminals to manipulate the will of a person is ϒ-hydroxybutyric acid (GHB) that can be introduced into the victim's drink without the victim being aware of it because it is a colorless, odourless and almost tasteless liquid. In addition, the effect after its intake is fast (15-30 min), lasts for periods of 6 to 8 hours and its detection is challenging because is quickly metabolized. Therefore, the preparation of colorimetric or fluorescent chemosensors to detect GHB is an active research field. Previous chromo-fluorogenic chemosensors able to detect GHB were either based on borodipyrromethene derivatives[1], enzymes coupled with a redox active dye[2] or cucurbiturils with fluorescent dyes[3]. In the present work, two new oxazole derivatives, **1** and **2** (see Scheme 1), able to detect ϒ-hydroxybutyric acid (GHB) in soft drinks and alcoholic beverages are presented. DMSO 10 µM solutions of both probes experience a clear color change from yellow to red easily detectable by naked-eye in presence of GHB (limit of detection of 0.13 and 0.12 µM, respectively) and in the case of probe **2**, also a marked emission enhancement at 541 nm (excidetation at 490 nm) is observed. A further study of the response of probe **1** in the presence of different beverages was also tested which conformed its usefulness in a real scenario.

The mechanism associated with the GHB detection of the probes was studied by UV-Vis titrations and ^{1}H NMR spectroscopy. The data obtained pointed to a single equilibrium between probe **1** andGHB linked to a upfield shift of all signals of the aromatic protons. This fact, consistent with an increase in the electron density of the probe as a consequence of the recognition process, was also supported by theoretical DFT calculations where the acidity of the amino group bearing the nitrophenol and fluorescein substituents was evaluated and the UV-Vis plots were predicted, pointing to the GHB-induced deprotonation of the probes as the reason of the chromo-fluorogenic response[4].

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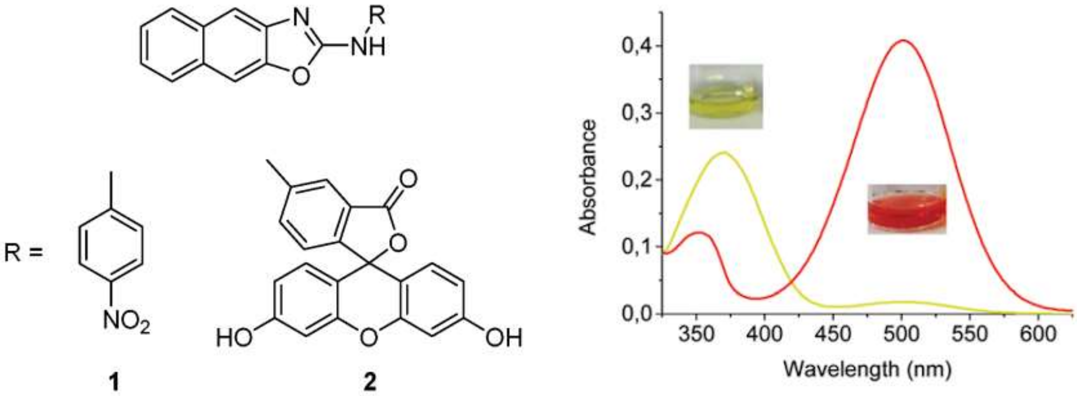

Figure 1: Chemical structure of oxazoles for GHB detection and UV-Vis spectra of probe **1** alone (yellow line) and in the presence of GHB 10 µM (red curve) in DMSO.

Phosphotungstate Nanoclusters enhance the capacitance and energy density of activated carbon in organic electrolyte supercapacitors

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Abstract

Phosphotungstic acid is a solid acid with reversible electroactivity and as such, we have previously shown how it can work as a faradaic additive to activated carbon (AC) in acidic aqueous electrolytes[1]. Yet, their use in organic media allows not only for added capacity but also higher voltage. We will present our recent work showing how the tetraethylammonium derivative of phosphotungstate $[PW_{12}O_{40}]^{3-}$ (PW12) can be homogeneously distributed throughout the pores of activated carbon (AC) in organic solvents such as N,N'-dimethylformamide (DMF) and demonstrate the use of this hybrid electrode material in an organic electrolyte (1 M TEABF4 in acetonitrile) supercapacitor. Our results show the efficient electroactivity of the PW12 cluster even in the absence of protons, providing a higher voltage than aqueous electrolytes and fast and reversible redox activity. The hybrid material shows a combination of double-layer (AC) and redox (PW12) capacities leading to an increase (36%) in volumetric capacitance with respect to pristine AC in the same organic electrolyte (1 M TEABF4 in acetonitrile)[2]. Remarkably, we were able to quantify this increase as coming predominantly from non-diffusion-limited processes thanks to the small size (1 nm) and utterly dispersed nature of these polyoxometalate (POM) clusters[2]. Moreover, the hybrid material delivers a good rate capability and excellent cycle stability (93% retention of the initial capacitance after 10,000 cycles). This study has a profound significance on improving capacitance of carbon-based materials in organic electrolytes.

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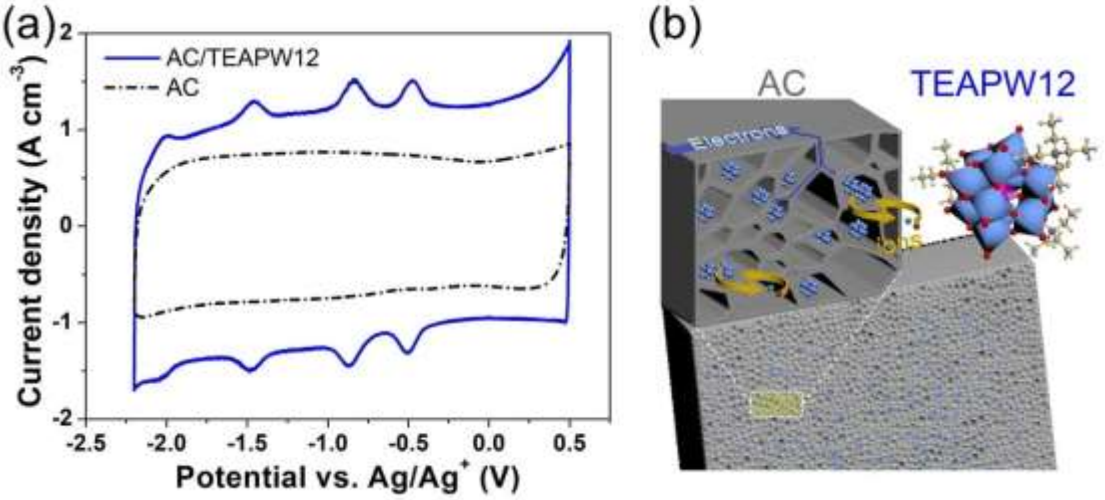

Figure 1: a) Cyclic voltammograms of AC and AC/TEAPW12 at 20 mV s^{-1} in three-electrode configuration, b) Schematic diagram of how the anchoring of TEAPW12 on AC allows for fast and reversible redox activity.

FLASH POSTERS

Continuous-flow synthesis of high-quality few-layer antimonene hexagons

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A novel family of layered materials from group-15 of the Periodic Table, called Pnictogens (P, As, Sb and Bi) have gained increasing attention due to their semiconducting behaviour, with thickness-dependent band gaps that can be modulated by strain, doping or chemical functionalization, which can be useful for fabricating optoelectronic devices. Additionally, these 2D-Pnictogens offer unique photonic, catalytic, magnetic, and electronic properties. [1] Within this chemical group, antimonene is a monoatomic 2D material with a buckled structure showing exceptional physico-chemical properties. Although some of its theoretically-predicted remarkable properties have already been experimentally demonstrated, others remain a challenge to corroborate because of the absence of a suitable synthetic method to produce the required high-quality material. [2] Antimonene can be isolated using top-down and bottom-up approaches. On the one hand, top-down methods such as micromechanical or liquid phase exfoliation have demonstrated the ability to produce limited lateral dimensions and partially oxidized hexagonal antimonene nanoflakes. [3] On the other hand, bottom-up methods as well as molecular beam epitaxy and van der Waals epitaxy approaches, have led to high-quality antimonene flakes but are not suitable for large-scale synthesis. [4] Another bottom-up approach has been recently reported, involving a solution phase synthesis of well-defined hexagonal few-layer antimonene via anisotropic growth, [5] which has facilitated large-scale production of this material. In this context, we optimized the synthetic parameters for the production of high quality few-layer antimonene hexagons, and their implementation in a large-scale manufacturing process under continuous-flow conditions to pave the way for optoelectronic device fabrication.

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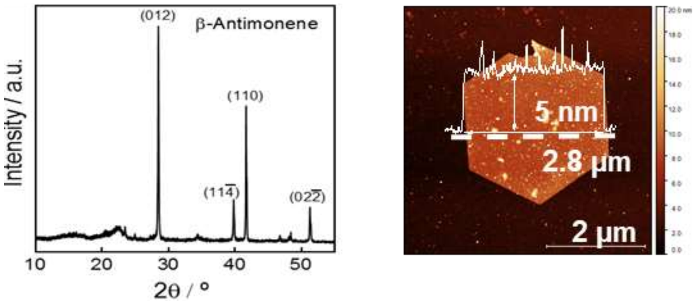

Figure 1: X-ray powder diffraction (left) and atomic force microscopy image (right) of hexagonal antimonene nanosheets synthesized using a colloidal chemistry approach.

Carborane Based π- Conjugated Systems for Two Photon Absorption (TPA)

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Abstract

The two-photon absorption (TPA) process is a third-order nonlinear optical (NLO) process in which materials simultaneously absorb two photons. Acceptor-Donor-Acceptor (A-D-A) or Donor-Acceptor-Donor (D-A-D) materials usually exhibit large two-photon cross section that can be applied like 3D optical data storage, optical limiting, microfabrication, photodynamic therapy or imaging. [1]
Icosahedral 1,2-dicarba-*closo*-dodecacarboranes or *o*-carboranes have highly polarizable spherical aromaticity through σ-delocalized electron densities.[2] Consequently, they display characteristic electronic properties as well as thermal, chemical and photochemical stability. These features make them interesting systems, especially for luminescent materials.[3],[4],[5] Carborane clusters, usually have a significant impact when attached to larger functionalities, acting as electron-acceptor groups linked through the carbon cluster. Thus, we aimed to prepare acceptor-donor type of systems containing *o*-carborane as an acceptor group. To this purpose, insertion reaction of decaborane ($B_{10}H_{14}$) into the acetylene precursors of fluorophores was performed (Figure 1). Therefore, a set of *o*-carborane based π-conjugated systems have been synthesized and characterized by usual techniques such as FT-IR and ^{1}H, ^{13}C and ^{11}B NMR spectroscopy. Furthermore, their photophysical properties (absorption and emission spectra) were analysed. Their potential TPA properties might lead to a prospective application in biomedicine, especially in super-resolution fluorescence microscopy and also in optical limiting.

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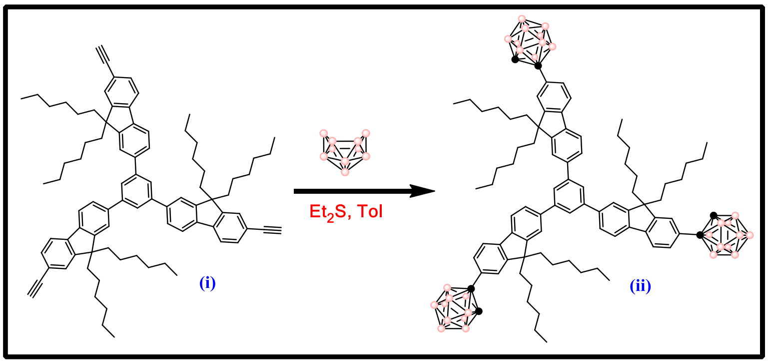

Figure 1: Preparation of carborane based π-conjugated system by insertion reaction.

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