S18 Nanoscience and Molecular Materials
Nanociencia y Materiales Moleculares (GENAM)

12/07 Tuesday afternoon, Aula 1.5 bis

15:30-16:00 José J. Baldoví Jachán (ICMol-Universidad de Valencia)
Tailoring magnetism in low-dimensional materials

16:00:16.30 M. José Martínez Pérez (INMA CSIC-Universidad de Zaragoza)
Ultrasensitive magnetic characterization at the nanoscale: from molecules to complex magnetic states

16:30-16:45 Enrique Burzurí Linares (Universidad Autónoma de Madrid)
Spin-state-dependent electrical conductivity in single-walled carbon nanotubes encapsulating spin-crossover molecules

16.45-17:00 Giancarlo Franzese (Universidad de Barcelona)
Uniqueness of water compared with other liquids under nano-confinement

17:00-17:15 Saúl Sánchez González (Universidad de Oviedo)
Relevance of Shockley states on the electrical and thermoelectric response of gold-based single-molecule junctions

17:15-17:45 **Posters and Coffee**

17:45-18:15 Miguel Anaya Martín (Cambridge University)
Molecular treatment in halide perovskites for next generation optoelectronic device

18:15-18:30 Arantxa Fraile Rodríguez (Universidad de Barcelona)
Multifunctional Plasmonic Nanostructures with 3-fold Symmetry

18:30-18:45 Pablo de Vera Gomis (Universidad de Murcia)
Charged-particle electronic cross sections in biomaterials: towards a detailed modelling of nanoscale biodamage

18.45-19:00 Gabriel Martínez Carracedo
Accurate exchange constants for bilinear-biquadratic spin models: application to graphene nanostructure

19:00-19:15 Julia García Pérez (IMDEA)
Electro-optical study of a MoS2 micro-drum resonator

19:15-19:30 Alberto M. Ruiz (Universidad de Valencia)
Chemical tailoring of the magnetic properties of two-dimensional materials

Posters:

18 Bruno Cosio Corujo (Universidad de Oviedo)
Study of edge states and topology on 2D flakes of dichalcogenides

19 Gabriel Caballero Catalán (IMDEA)
Electrical properties of mechanically exfoliated MoS2 devices under different ambient conditions

20 Alberto Montoya Ruiz (ICMol-Universidad de Valencia)
Tailoring the magnetic properties of 2D magnetic materials

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Spin-state-dependent electrical conductivity in single-walled carbon nanotubes encapsulating spin-crossover molecules

Aysegul Develioglu[1], Julia Villalva[1], Nicolas Montengro-Pohlhammer[2], Rocío Sánchez de Armas[2], Mar García-Hernandez[3], Jose Sánchez-Costa[1], Carmen J. Calzado[2], Emilio M. Pérez[1], **Enrique Burzurí**[4,1,*]

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Mixed-dimensional heterostructures [1] combine materials of different dimensionality (0D, 1D, 2D…) to create hybrid materials in which some limitations casted by a specific dimensionality can be overcome.

One of these examples are spin crossover (SCO)-based materials. SCO molecules are promising nanoscale magnetic switches due to their ability to modify their spin state under several stimuli. However, SCO systems face several bottlenecks when downscaling into nanoscale spintronic devices: their instability at the nanoscale, their insulating character and the lack of control when positioning nanocrystals in nanodevices. Here we show the encapsulation of robust Fe-based SCO molecules within the 1D cavities of single-walled carbon nanotubes (SWCNT) [2]. We find that the SCO mechanism endures encapsulation and positioning of individual heterostructures in nanoscale transistors. The SCO switch in the guest molecules triggers a large conductance bistability through individual host SWCNT. Moreover, the SCO transition shifts to higher temperatures and displays hysteresis cycles, and thus memory effect, not present in crystalline samples. Our results demonstrate how encapsulation in SWCNTs provides the backbone for the readout and positioning of SCO molecules into nanodevices, and can also help to tune their magnetic properties at the nanoscale.

Alternatively, we explore additional methods to bond magnetic molecules to 1D SWCNTs [3]. I will introduce the mechanical bond that has allowed us to embrace magnetic porphyrin dimeric rings around carbon nanotubes without disturbing their mutual properties. Spin coherence times of the order of microseconds are found in these mixed-dimensional heterostructures, positioning them for quantum computing.

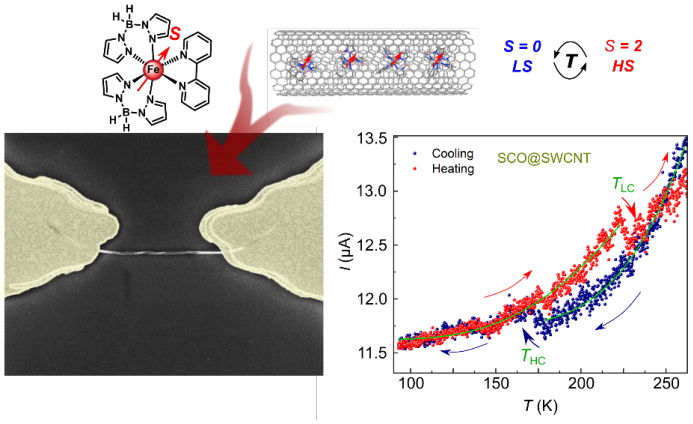

Figure 1. Encapsulation of SCO molecules within 1D SWCNT produces a distinct conductance bistability in the host SWCNT and a modification of the SCO properties in the guest molecule

[1] D. Jariwala, T. J. Marks and M. C. Hersam, *Nature Materials* **16**, 170 (2017).
[2] J. Villalva, A. Develioglu, […], E. Burzurí, *Nature Communications* **12**, 1578 (2021).
[3] S. Moreno-Da Silva, J. I. Martínez […] E. Burzurí, *J. Am. Chem. Soc.* **143**, 21286 (2021).

Uniqueness of water compared with other liquids under nano-confinement

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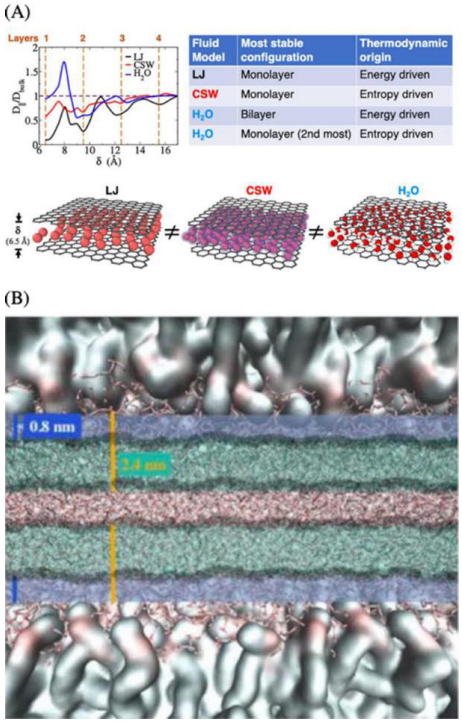
Living organisms, viruses, and technological devices have water layers between their cells or parts and can die or stop working when dehydrated. But why water and not any other fluid? What makes water unique when it is in these tiny pores? We investigate why the water in a pore tinier than one-millionth of a hair moves faster than free water, while other fluids do not. We show that it all depends on the peculiar hydrogen bond interaction of water [1] (Fig. A). The results might be a key factor contributing to the solution of the United Nations Sustainable Development Goals about clean water and sanitation and relate to the switching behavior observed in a hydrated graphene nano-memristor proposed as a memory device that could store the data of 100 trillion flash memories in just 1 cm^3 for quantum computing [2, 3].

On the other hand, water's uniqueness is also essential in cellular membranes. We revise and extend the concept of 'hydration' or 'biological water', i.e., the nanoscopic layer of water covering the surface of biosystems. We find and discuss the existence of a bound/unbound water interface and its effect on dynamics and structure as far as 2.4 nm away from the membrane (Fig. B). The results might be relevant for understanding the role of water in biological activity, e.g., the efficacy of new drugs or vaccines [4, 5, 6].



(A) Comparison of the diffusion of a normal fluid (LJ), an anomalous fluid (CSW), and water in a graphene nanopore. Their free energies change differently with the pore size (upper right table), and water is the only one that diffuses faster than bulk under sub-nm confinement (upper left panel). (B) Atomistic simulations of water between two membrane leaflets, Martelli et al. (2021). Away from the lipids (smooth surfaces), we schematically mark three regions: lipid-bound water (blue), unbound water (green), bulk water (red and withe stick molecules), and the interfaces between them (dark regions). Water penetrates between the lipids and persists there even at low hydration.

Referencias

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[2] H-T. Chin, et al. *Ferroelectric 2D ice under graphene confinement*, Nat. Commun. **12**, 6291 (2021).

[3] G. Franzese, *Supercomputer memories made of water*, https://doi.org/10.32388/9NTVN5.

[4] F. Martelli, J. Crain, and G. Franzese, *Network Topology in Water Nanoconfined between Phospholipid Membranes*, ACS Nano **14**, 8616 (2020).

[5] F. Martelli, C. Calero, and G. Franzese, *Redefining the concept of hydration water near soft interfaces*, Biointerphases **16**, 020801 (2021).

[6] The work has been possible thanks to the financial support of the Spanish MICIN grant PGC2018- 099277-B-C2, the ERDF (A way of making Europe), and the ICREA - Institució Catalana de Recerca i Estudis Avançats.

Relevance of Shockley states on the electrical and thermoelectric response of gold-based single-molecule junctions

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Noble metals break preferably exposing (111)-oriented surfaces, that host Shockley type surface states (Sss) [1]. Nevertheless, the relevance of SSs on the electrical properties of gold-based molecular junctions has not been explored in detail. Here, we present ab-initio simulations that show how the gold (111) SS, that lies approximately 0.5 eV below the Fermi energy, is key to determining correctly the electrical and thermoelectric response of the above junctions. We also show that gold's SS appears in our simulations only if d-orbitals are included explicitly in the valence shell. We discuss in detail Benzenediamine (BDA) and Benzenedicarbonitrile (BDCN) gold (111) junctions, where we also include the DFT+Σ correction scheme [2].

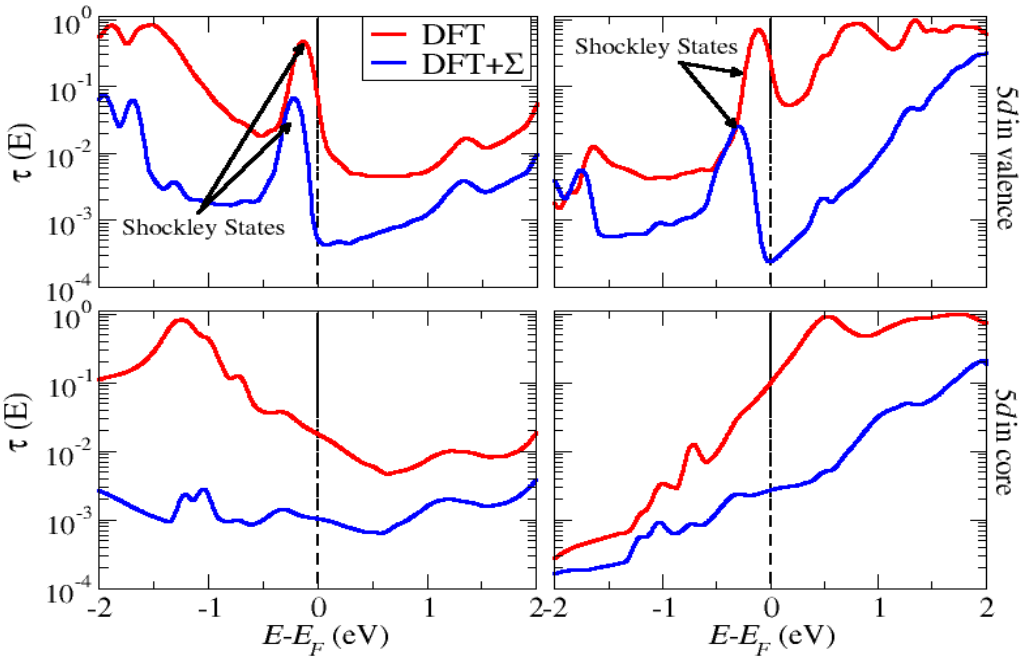

Figure 1. Transmission function of BDA (left panels) and BDCN (right panels). Top (bottom) row corresponds to the junctions where gold's 5d orbitals are explicitly included in the valence (core) shell. The intersection between the graphs and the vertical lines gives the low-voltage conductance. The slope of the transmission function at the Fermi energy is proportional to the thermopower.

[1] Yan, B., Stadtmüller, B., Haag, N. et al., *Nat. Commun,* **6**, 10167 (2015).
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Multifunctional Plasmonic Nanostructures with 3-fold Symmetry

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In this contribution we present the results of our work with structures that follow 3-fold symmetry designs. These structures present a high degree of geometric frustration due to the fact that plasmonic resonances ultimately rely in the excitation of charge oscillations in the nanostructure and a dipolar excitation cannot be easily accommodated into a 3-fold symmetry. Taking advantage of this feature, several structures exhibiting narrow resonance and the appearance of high energy modes have been studied. We will discuss two of them.

The first is a refractive index sensor based on the excitation of collective excitations in an Au inverted honeycomb plasmonic lattice [1]. Due to its high sensitivity to changes in the surrounding medium, this sensor was able to show sensitivity values ranging from 99 to 395 nm/RIU (RIU stands for refractive index unit) for relatively thin layers of test materials within 50 and 200 nm. The structure was manufactured by a method based on electron beam lithography and the measured optical response agreed with the simulations.

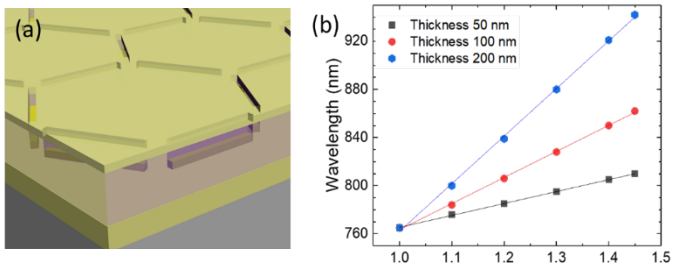

Figure 1. (a) Schematic representation of the structure. (b) Wavelengths of the plasmonic resonance as a function of the refractive index for three values of the test layer thickness.

Our second work is focused on the design and simulation of a simple 3D structure that presents large CD in the near-Infrared (NIR) and optical ranges that can be easily tuned by adjusting its geometrical parameters [2]. Our simulations reveal that the stacked triskelia system present a strong dichroic signal in the extinction. The arising dichroism is mainly due to two extra excitations, not present in the single element case, exhibited by the absorption at wavelengths greater than 0.7 and 1.1 μm, respectively. Furthermore, the position of these two peaks can be shifted by changing either the edge-to- edge distance between the triskelia or their relative angle of rotation. This strongly supports the fact that these additional excitations are caused by the interactions between the two triskelia. Such shifting enables an accurate control of both the wavelength ranges at which the CD appears and its sign, by adjusting the distance between the triskelia and their relative rotation angle, two parameters that can be easily tuned in the manufacturing process.

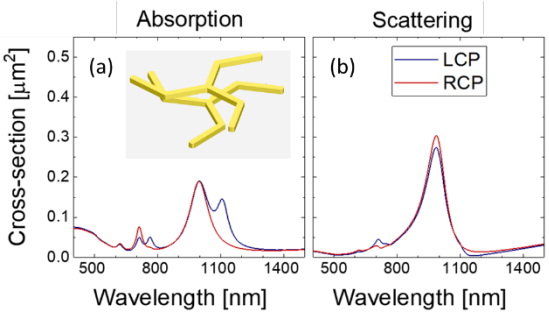

Figure 2. Absorption (a) and scattering (b) cross-section spectra for the stack of two triskelia for right- and left-handed circularly polarised light. The twist angle is 30°.

[1] J. Rodríguez-Álvarez et al., *Nanomaterials* **11**, 5 (2021).
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Charged-particle electronic cross sections in biomaterials: towards a detailed modelling of nanoscale biodamage

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The biological effects of radiation, in terms of cell killing or inactivation, are determined by the damage patterns that the beam particles induce on the nanometre scale. This is particularly true for the swift ions used in the modern ion beam cancer therapy, whose enhanced relative biological effectiveness cannot be explained in terms of macroscopic energy deposits, but it is only understood once the clustering of damaging events on the length scales of the DNA molecules are considered [1]. Swift ions produce numerous very-low energy (<50-100 eV) secondary electrons, which travel distances of a few nanometres around the ion's paths, producing large concentrations of inelastic events in the sensitive biomolecules (Fig. 1).

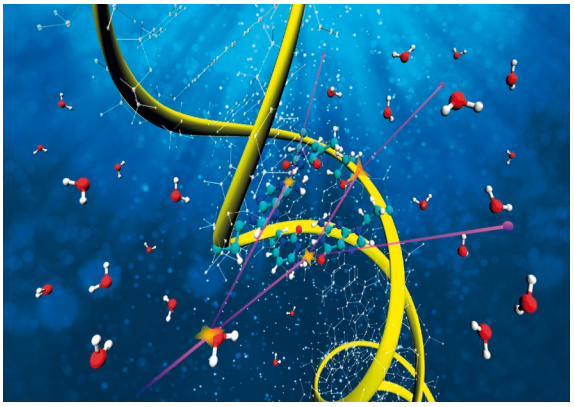

Figure 1. Artistic illustration of the interaction of low energy electrons with DNA in liquid water [7].

The modelling of the energy deposition on the nanoscale is very sensitive to the set of interaction probabilities (cross sections) between charged particles and the relevant biomolecular materials, including liquid water (the main constituent of living tissues) and the building blocks of DNA (bases and backbone), among other biomaterials. The main channel leading to charged-particle energy loss is electronic interactions, and both ionisations (releasing electrons) and electronic excitations (leading to local energy deposits) need to be considered in order to accurately model the nanometric track-structure of ion beams. However, current Monte Carlo simulation codes for radiation transport in biomaterials, such as Geant4-DNA [2], can only describe, up to date, the interaction of charged particles with liquid water, which limits their accuracy.

Over the recent years, in our research group we have exploited the theoretical framework known as the dielectric formalism [3], based on the first Born approximation (FBA), to develop a series of methods to obtain electronic excitation and ionisation cross sections, both integral and differential (in secondary electron ejection energy and angle), for arbitrary biomaterials. These models were first introduced for the impact of ion beams [4,5], to be more recently extended for electron beams by including their particularities in terms of low energy corrections to the FBA and electronic exchange [6,7]. The purpose of this contribution is to review these methods, and to show the general good agreement between theory and experiments got for both ions and electrons in a wide energy range and for a large collection of relevant biomolecular materials. These models and cross sections will be very useful to advance towards a detailed modelling of nanoscale radiation biodamage.

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[3] I. Abril, R. Garcia-Molina, C. D. Denton, F. J. Pérez-Pérez, N. R. Arista, *Physical Review A* **58**, 357 (1998).
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Accurate exchange constants for bilinear-biquadratic spin models: application to graphene nanostructure

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We propose a new method to determine accuarately the exchange constants of long-range Heisenberg bilinear-biquadratic models (BLBQ). The method uses Hamiltonians and overlap matrices given by DFT calculations within the framework of non-orthogonal basis sets [1,2] . We also compare the results given by this method with the experimental results for triangulene graphene nano-structures making up quantum spin chains (TSCs) [3]. These are S=1 chains and hence exotic phenomena like the Haldane phase arise [4, 5]. We also propose possible experimental settings to change the ground state of finite-length TSCs from a singlet to a triplet. We determine via a combination of exact Diagonalization and DFT calculations (ED) ways to control the above singlet-triplet transition.

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Electro-optical study of a MoS_2 micro-drum resonator

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Nanoelectromechanical systems (NEMS) are a sort of device capable of transducing an electrical signal to a mechanical motion or in reverse. In particular, drum resonators based on two-dimensional materials have been thoroughly studied in the last few years due to their mechanical properties and potential applications, such as sensors [1]. In this work, we study the electrical and optical properties of micro-drum resonators fabricated with mechanically exfoliated MoS_2.

First, we use maskless optical lithography to deposit Ti/Au electrodes onto a SiOx/Si substrate. These will be used for the electrical actuation of the resonators. To fabricate the NEMS, we mill 5 µm-wide, 500 nm-deep holes between the electrodes with a Focused Ion Beam (FIB) tool. Then, we deterministically transfer a few-layer molybdenum disulfide (MoS_2) flake onto the hole, fully covering it and bridging the two electrodes [2].

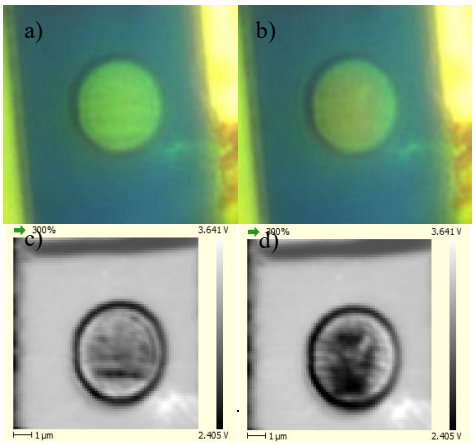

Figure 1. Images of the device at a) V_{DC} = 0V and b) V_{DC}= 40V. Relative reflectance images of the microdrum at c) V_{DC} = 0V and d) V_{DC}= 40V.

By applying DC and RF electric fields between the top electrodes and the bottom of the covered hole we induce mechanical oscillations in the suspended region, studying the resonant membrane's motion at the nanoscale under different tensile strain conditions. Readout of the mechanical movement of the membrane is performed via changes in the system's reflectivity by focusing a laser onto the surface of the suspended region of the flake with a high NA objective. We study the electro-mechanical response of the drum resonator both at atmospheric pressure and in high-vacuum, in this last case, at room temperature and cryogenic conditions. We observe the evolution of the fundamental mode, the first vibrational harmonic and their transition from the linear to the non-linear regime under different excitation conditions [3].

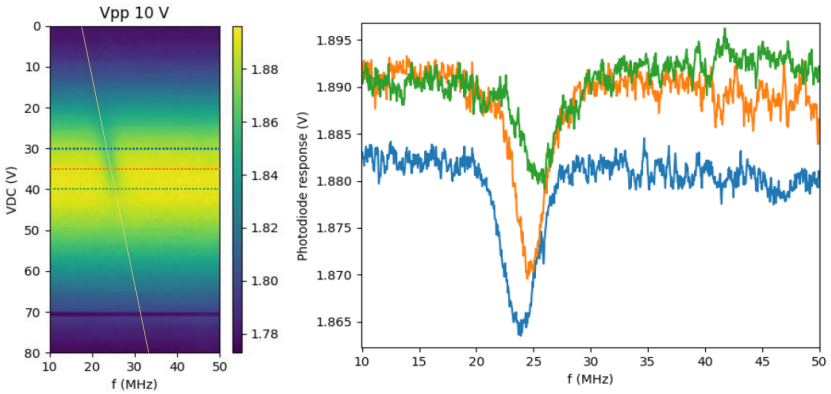

Figure 2. Optical response of a MoS_2 drum resonator at atmospheric pressure subjected to a RF sweep versus different amplitudes of the applied V_{DC}. The frequency of the fundamental mode changes linearly with the applied V_{DC}.

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Edge states and topology in dichalcogenides nanostructures

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The study of 2D-materials has been promising since the popularization of graphene. Transition Metal dichalcogenides display a number of interesting electronic and optical properties, where the role of the Spin Orbit interaction is also enhanced.

We show our recent work on diverse nano-structures of the Transition Metal dichalcogenide MoS2 whose electronic structure has been elucidated recently via SPM probes [1,2].

We analyse the emergence and robustness of edge states and look specifically on their possible topological protection via Tight Binding modelling and downfolding. Some of the analysed regular nanostructures have been synthesized already while a few others have not, raising the possibility to identify new types of edge states.

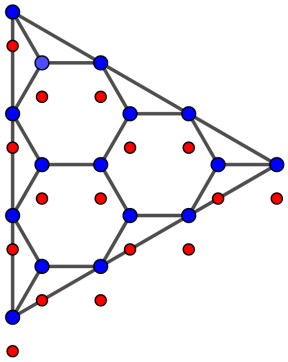

Figure 1. Flake structure of MoS2 with blue dots as the Mo atoms and the red ones as S.

[1] Mark J. Haastrup, Mathias H. R. Mammen, Jonathan Rodríguez-Fernández, and Jeppe V. Lauritsen, Lateral Interfaces between Monolayer MoS2 Edges and Armchair Graphene Nanoribbons on Au(111), *ACS Nano* **15**(4), 6699 **(**2021).

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Electrical properties of mechanically exfoliated MoS_2 devices under different ambient conditions

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2D-layered materials such as graphene and transition metal dichacogenides (TMDs) are promising due to their unique electrical, optical and mechanical properties, and their possible applications in electronic, optoelectronic and quantum computation devices.

In this work we focus on the study of 3 terminal field-effect transistor devices, based on mechanical MoS_2 flakes mechanically exfoliated on top of SiO_2/Si substrates. We have characterized the structural properties od MoS_2 devices by means of AFM (Atomic force Microscopy) and Ramana spectroscopy. We will present current-voltage characteristics (I_{SD} vs V_{SD}) and transfer characteristics (I_{SD} vs V_G) performed under ambient and vacuum conditions and at room and low temperature [1,2].

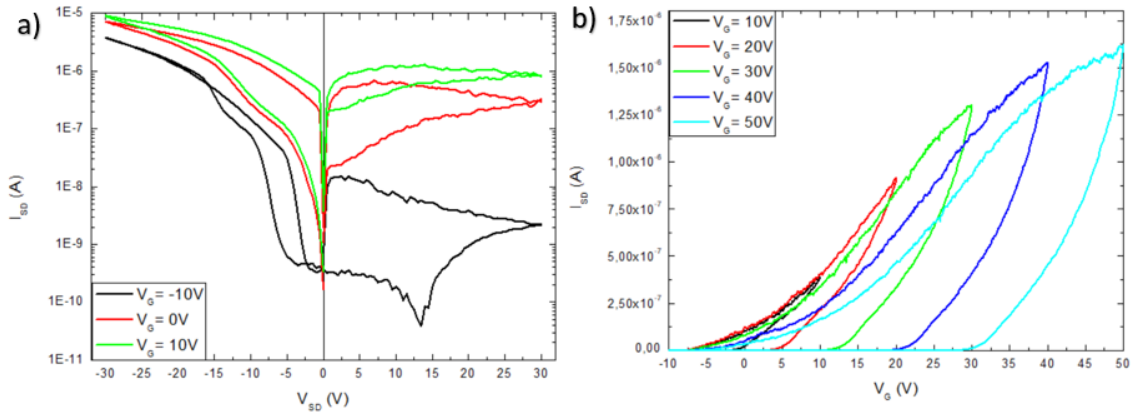

Figure 1. (a) Transfer characteristics (I_{SD} vs V_G) at constant source-drain voltage V_{SD}=1V. (b) Current-voltage characteristics (I_{SD} vs V_{SD}) at different back-gated voltages; V_G= -10 V (black), V_G = 0 V (red) and V_G = 10 V (green).

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Chemical tailoring of the magnetic properties of two-dimensional materials

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The recent discovery of two-dimensional (2D) magnets has provided an unexplored and ideal platform to manipulate and control 2D magnetism and thus having applications in spintronics, magnonics, data storage or quantum computing, among others [1]. CrSBr is a Van der Waals magnetic material, recently isolated to the monolayer limit. It presents a ferromagnetic character with spins pointing in plane, with a curie temperature (T_c) of 145 K [2] and lattice evolution as one cools down below this temperature tends to maximize ferromagnetic interactions along the four different exchange paths [3]. However, a deeper magneto structural study of this material is still lack, relating how magnetic properties change under Coulombic screening and strain modifications.

In this talk we present the theoretical results obtained for the CrSBr monolayer and its structural and electronic properties based on density functional theory (DFT) as implemented in the Quantum Espresso code [3]. By constructing a tight-binding Hamiltonian based on maximally localized Wannier functions (MLWFs), as implemented in the Wannier90 package [4], we could describe the system by choosing *d* orbitals of Cr and *p* orbitals of both S and Br. At this stage, Green functions are used to construct a Heisenberg Hamiltonian to obtain information about the magnetic exchange interactions, as implemented in the TB2J code [5]. Finally, we studied the deposition of organic planar molecules in order to analyse proximity effects between them and CrSBr, through the structural and electronic properties of the resulting heterostructures. This will pave the way for further understanding of the deposition of different molecules that can induce local-strain effects in 2D materials.

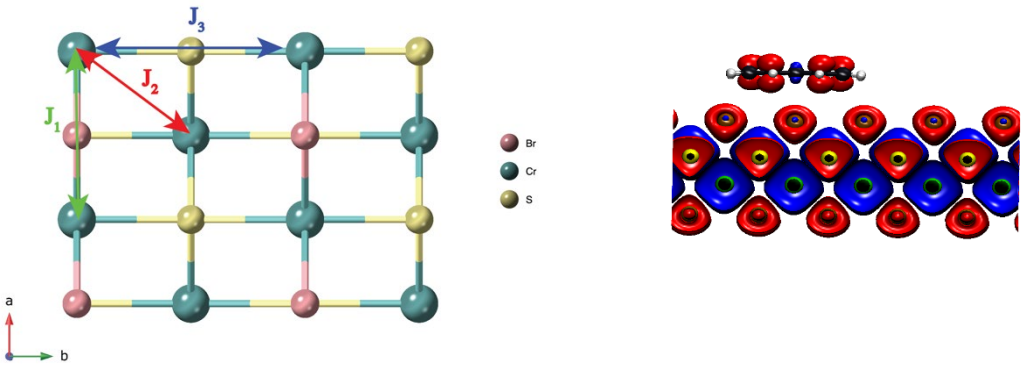

Figure 1. Top view of CrSBr monolayer pointing the J_1, J_2 and J_3 directions (left), spin density of a hybrid heterostructure formed by CrSBr monolayer and an organic molecule (right).

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