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The conference will take place from **July 8 to 11, 2025**, at the **Palacio de congresos of Oviedo**. Renowned speakers will present on key topics including atomic force microscopy, scanning tunneling microscopy, and theoretical aspects of scanning probes. We invite you to join us at FyT 2025 to explore the latest breakthroughs in scanning probes and connect with the Spanish SPM community while experiencing the stunning natural surroundings of Oviedo.

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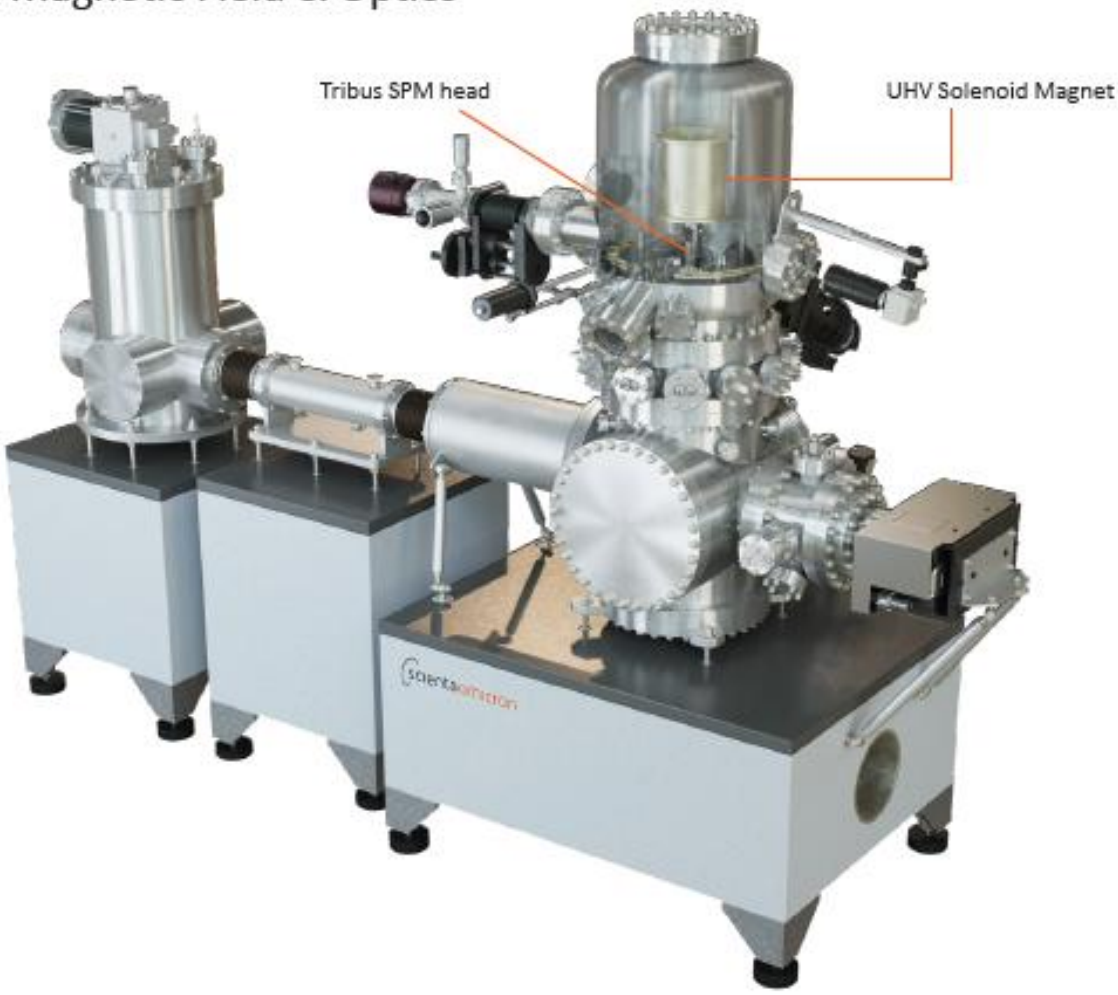

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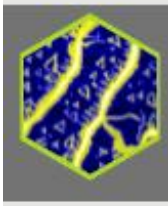

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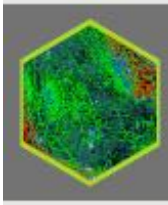

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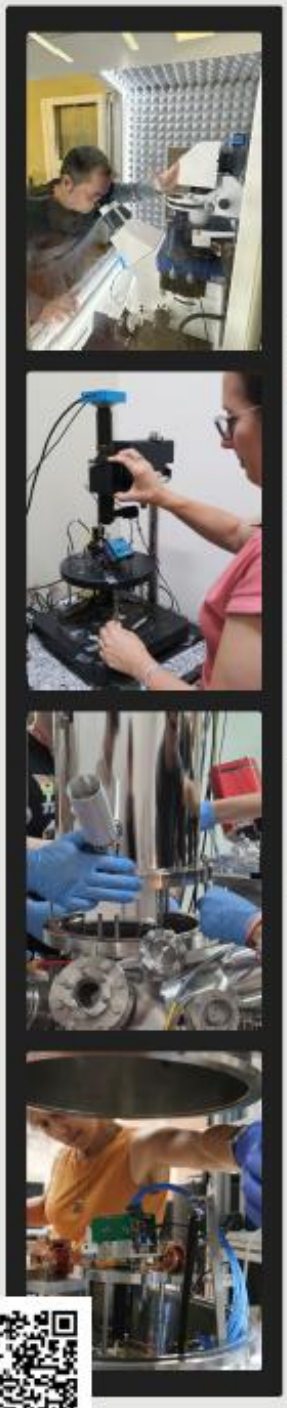

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Borja Cirera, Materials Science Institute of Madrid (ICMM-CSIC), Spain

Program

Tuesday 8th

18:00	**Registration opens**

Session chair: Esther Barrena	
18:30	**Opening**
19:00	**Pablo Alonso** (Universidad de Oviedo, Spain) *Light and molecules at the nanoscale*

20:00	**Welcome cocktail**

Wednesday 9th

Session chair: David Ecija	
9:00	**Jeppe Lauritsen** (Interdisciplinary Nanoscience Center, Aarhus University, Denmark) *Catalysis Insight from Scanning Probe Microscopy: From Metal Oxides to Single Atoms in Carbon Nitrides*
9:45	**Sergio Jiménez-Fernández** (Instituto de Ciencia de Materiales de Madrid, Spain) *Formation of the surface alloy Au2Sn driven by hydrogen etching of β-SnSe/Au(111)*
10:00	**Kevin García Díez** (Catalan Institute of Nanoscience and Nanotechnology (ICN2), Spain) *Electronic properties of Bismuth monolayers on metallic substrates*
10:15	**Jesús Redondo** (Charles University, Czech Republic) *Unveiling the surface of model and realistic copper sulfides*
10:30	**Adrián Sáez-Coronado** (Instituto de Ciencia de Materiales de Madrid, Spain) *Synthesis and characterization of a two-dimensional ionic hydride*
10:45	Coffee break
Session chair: Ana Sánchez-Grande	
11:15	**Eva Osuna** (Universidad Autónoma de Madrid, Spain) *Unveiling the Origin of the Scale-Dependent Conductivity of Ni3(HITP)2 Metal-Organic Framework Thin Films*
11:30	**Borja Cirera** (Instituto de Ciencia de Materiales de Madrid, Spain) *Atomic Precision Mapping of Site-Specific Vibrations in Single Molecules*
12:00	**Miguel Varea** (IMDEA Nanociencia, Spain) *Light-matter interaction of field emission resonances in a scanning tunneling microscope*
12:15	**Andrés Pinar Solé** (Center for Quantum Nanoscience, Korea) *Site-Specific Charge of a Ho atom on MgO*
12:30	**Benjamín Mallada** (Institute of Physics, Czech Academy of Sciences, Czech Republic) *Real-space imaging of π-holes*
12:45	**Benjamin Lowe** (Institute of Physics, Czech Academy of Sciences, Czech Republic) *Open-shell character and charge-state control of an organic macrocycle on Au(111) and semiconducting FeCl2*
13:00	Lunch
Session chair: Eider Berganza	

14:30	**Ana Pérez-Rodríguez** (Universidad de Salamanca, Spain) *Nanoscale Electrostatics in Thin-Film Transistors: from Organic Semiconductors to 2D TMDs*
15:00	**Esther Calle** (Instituto de Ciencia de Materiales de Madrid, Spain) *Dielectrophoresis as a tool for investigating magnetic and transport properties of single magnetic nanowires by Magnetic Force Microscopy*
15:15	**Pablo Martínez Outomuro** (Instituto de Ciencia de Materiales de Madrid, Spain) *Roughness induced magnetic domains changes in CoFeB/Pd multilayers*
15:30	**Jorge Marqués-Marchán** (Instituto de Ciencia de Materiales de Madrid, Spain) *Customizing Magnetic Force Microscopy probes: going beyond standard imaging*
15:45	**Diego A. Aldave** (Universidad Autónoma de Madrid, IFIMAC, Spain) *Magnetic field screening of 2D materials revealed by magnetic force microscopy*
16:00	Coffee break
Session chair: Nacho Martínez	
16:30	**Mario Navarro-Rodríguez** (Universidad de Murcia, Spain) *Porphyrin-GO nanohybrids: insights into morphological, optical, and electronic properties at the nanoscale*
16:45	**Daniel Gallego-Fuente** (Universidad Autónoma de Madrid, Spain) *A versatile technological UHV-compatible AFM: adhesion and friction mapping in Ultra High Vacuum*
17:00	**Carlos Romero-Muñiz** (Universidad de Sevilla, Spain) *Tautomerization processes and molecular defects revealed by scanning probe microscopy and first-principles calculations*
17:30	**Aurelio Gallardo** (IMDEA Nanociencia, Spain) *Computational characterization of low-dimensional molecular nanostructures and their SPM imaging*
17:45	**Jara Trujillo-Mulero** (Universidad Autónoma de Madrid, IFIMAC, Spain) *Accurate forces for CO tips on cobalt phthalocyanines on Ag(111)*
18:00	**Oscar Mateos-Lopez** (Universidad Autónoma de Madrid, Spain) *Revisiting the formation of water nanomenisci*

Thursday 10th

Session chair: Pedro J. de Pablo	
9:00	**Wouter H. Roos** (Rijksuniversiteit Groningen, the Netherlands) *Nanoscale dynamics of biomolecular interactions: from viruses to antibiotics*
9:45	**Alejandro Díez-Martínez** (Universidad Autónoma de Madrid, Spain) *Through the Lens of Force: Deciphering Melbournevirus' Structural Secrets through Atomic Force Microscopy*
10:00	**E. M. Martín-Cuevas** (Spanish National Center of Biotechnology, Spain) *Structural Characterization of RNA combining AFM, Chemical Probing and Dynamic Fitting.*
10:15	**Beatriz Cantero Nieto** (Institute for Bioengineering of Catalonia, Spain) *Highthroughput Biomechanical Characterization of Macrophage Polarization Through Atomic Force Microscopy*
10:30	**Marko Grabarics** (University of Oxford, UK) *Atomically resolved imaging of the conformations and adsorption geometries of individual β-cyclodextrins with non-contact AFM*
10:45	Coffee break

Session chair:Aitor Mugarza	
11:15	**M. Cano** (Universitat de Barcelona, Spain) *Nanoscale dielectric imaging of cells and bacteria by scanning dielectric microscopy assisted by deep convolutional neural networks*
11:30	**Yu Kyoung Ryu** (Universidad Politécnica de Madrid, Spain) *Patterning of graphene and MoS2 devices by thermal scanning probe lithography*
12:00	**Aitor Zambudio** (Universidad Autónoma de Madrid, Spain) *2D Monolayer Tip Coating*
12:15	**Beatriz Viña-Bausá** (Universidad Autónoma de Madrid, Spain) *Controlling spin ½ interactions in graphene: from quantum entanglement to altermagnetism*
12:30	**Diego Expósito** (Universidad Autónoma de Madrid, Spain) *Newly developed UHV-LT-Transport-STM/AFM system. From macro to nano in 10 minutes*
12:45	**Héctor González-Herrero** (Aalto University, Finland) Atomically sharp 1D interfaces in 2D lateral heterostructures of VSe2-NbSe2 monolayers

13:00	Lunch

Session chair: Héctor González-Herrero	
14:30	**Antonio J. Martínez-Galera** (Universidad Autónoma de Madrid, Spain) *The synergy of scanning probe microscopy and 2D materials to advance nanocatalysis*
15:00	**Oscar Gutiérrez-Varela** (Instituto de Ciencia de Materiales de Madrid, Spain) *Frictional Contrast of Atomic Defects: A Combined LFM and MD Approach*
15:15	**Kyungmin Kim** (Osaka University, Japan) *Atomic-Scale Investigation of the CeO_2(100) Surface using Atomic Force Microscopy and Force Spectroscopy*
15:30	**Manuele González Lastre** (Universidad Autónoma de Madrid, Spain) *Identifying Ce3+ sites at the reduced CeO_2 (111) surface: the role of water molecules and AFM imaging*
15:45	**LMA**
15:55	**SPECS**
16:05	**Scienta Omicron**
16:15	**RHK**
16:25	**Scientec Iberica**

16:40-19:00	**Poster Session**

20:00	Conference Dinner

Friday 11th

Session chair: Pablo Ares	
9:00	**Laura Fumagalli** (University of Manchester, UK) *Unraveling the anomalous dielectric properties of interfacial and nanoconfined water*
9:45	**Jae Hwan Jeong** (Universidad Autónoma de Madrid, Spain) *Calibration of Scanning Joule Expansion Microscopy for nanoscale heat transport studies*
10:00	**Pranav Sudersan** (Universidad de Murcia, Spain) *Nanoscale wetting characterization using non-contact Scanning Probe Microscopy in humid conditions*
10:15	**Daniel Martín-Jimenez** (Institut de Ciència de Materials de Barcelona, Spain) *Bimodal atomic force microscopy with a torsional eigenmode for highly accurate imaging of grain orientation in organic thin films*
10:30	**Ignacio Horcas** (Universidad Autónoma de Madrid, IFIMAC, Spain) *Jumping Mode++ (Touch & Go)*

10:45 Coffee break

Session chair: Benjamín Mallada	
11:15	**Ana Sánchez-Grande** (Institute of Physics, The Czech Academy of Sciences, Czech Republic) *Photochemical reactions on a semiconducting surface*
11:45	**Ezequiel Tosi** (Instituto de Ciencia de Materiales de Madrid, Spain) *On-surface light vs thermal synthesis of a porous network*
12:00	**Sergio Salaverría** (Centro de Investigación en Nanomateriales y Nanotecnología, Spain) *On-surface synthesis and characterization of [19]-starphene*
12:15	**Federico Villalobos** (Universidad de Granada, Spain) *Globally aromatic odd-electron π-magnetic macrocycle*
12:30	**Eliecer Pelaez-Sifonte** (Instituto de Nanociencia y Materiales de Aragón, Spain) *Inducing radical states by nitrogen deprotonation in pyrrole bearing polycyclic hydrocarbons*
12:45	**Kalyan Biswas** (IMDEA Nanociencia, Spain) *Designing highly delocalized solitons by harnessing the structural parity of π-conjugated polymers*

13:00 Concluding remarks

Poster presentations:

Noor ul Ain Iqbal (IMDEA Nanociencia, Spain) *Unexpected 4x4 charge density wave in 1H-NbTe2 monolayer*	1
Rodrigo Arilla (Institut de Ciència de Materials de Barcelona, Spain) *Tapping-mode atomic force microscopy with high-order eigenmodes for true-molecular resolution in organic thin films*	2
Cosme G. Ayani (Center for Advanced Laser Techniques, Croatia) *VS_2 Epitaxy on Strained and Relaxed Graphene*	3
Jon Azpeitia (Instituto de Ciencia de Materiales de Madrid, Spain) *Physisorption or chemisorption: unveiling the nature of functionalized MoS_2*	4
Parmenio Boronat Sevilla (Institut de Ciència dels Materials de la Universitat de València, Spain) *Nano-surface photovoltage study of halide perovskite solar cells*	5
Víctor Camús (Universitat de València, Spain) *Co-localized KPFM & Raman scattering studies of graphene oxide reduction*	6
Roberto Carrasco (Universidad Autónoma de Madrid, Spain) *Twistraintronics: mechanical and electronic in-situ manipulation of magic angle graphene using STM*	7
Alba Cazorla (Instituto de Ciencias de Materiales de Barcelona, Spain) *Polar Crystalline order on asymmetric BTBT Derivatives revealed by Kelvin Probe Force Microscopy*	8
Jaime Colchero *(*Universidad de Murcia, Spain) *Torsional Mode Dynamic AFM as versatile multifrequency mode: challenges and possibilities*	9
Pedro J. de Pablo (Universidad Autónoma de Madrid, Spain) *New insights into tobacco mosaic virus: stability, disassembly and uncoating*	10
David Écija (IMDEA Nanoscience, Spain) *Generating antiaromaticity in polycyclic conjugated hydrocarbons by thermally selective skeletal rearrangements at interfaces*	11
Jose Manuel Filiu Samper (Universidad de Murcia, Spain) *A new modular Atomic Force and Optical Microscope as nanoLab*	12
Niklas Friedrich (University of Regensburg, Germany) *A chemical reaction triggered on ultrashort time scales with single-molecule selectivity*	13
Santiago Galán (University of Oviedo, Spain) *On-Surface Synthesis of (1,3)-chGNRs with Five-Membered Ring Edge Extensions*	14
Alba García Frutos (IMDEA Nanoscience) *Tailoring on-surface polymerization by molecular coverage through indenyl coupling*	15

Abstracts: Oral presentations

Light and molecules at the nanoscale

Pablo Alonso González [a,b]

[a] Department of Physics, University of Oviedo, Oviedo 33006, Spain.

[b] Center of Research on Nanomaterials and Nanotechnology, CINN (CSIC-Universidad de Oviedo), El Entrego 33940, Spain

* pabloalonso@uniovi.es

Recent experiments have discovered light at the nanoscale (polaritons) exhibiting strongly anisotropic propagation (hyperbolic) and extreme field confinement in 2D materials, such as α-phase molybdenum trioxide (α-MoO_3) [1]. In this talk, we will demonstrate that this exotic nanolight enables, for the first time, the visualization of directional-dependent strong coupling phenomena with organic molecules (pentacene) [2]. To support this claim, we will show near-field images taken by scattering-type scanning near-field optical microscopy (s-SNOM), which allow to directly corroborate the strong coupling variation as a function of in-plane angle. This result opens the door to several new applications such as directional sensing or directional local control of chemical properties at the nanoscale.

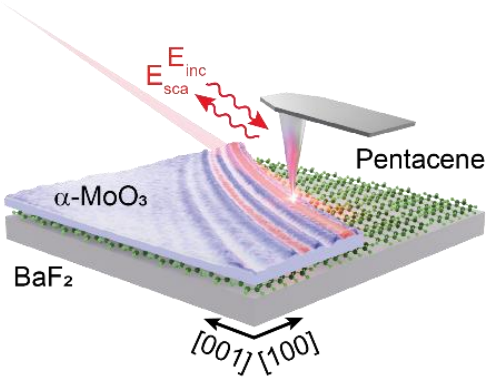


Figure - Schematic of the visualization by s-SNOM of strong coupling between polaritons and pentacene molecules.

References

[1] Ma, W. et al., Nature, 562, 557-562 (2018).

[2] Tresguerres-Mata, A.I.F. et al., (in revision).

Catalysis Insight from Scanning Probe Microscopy: From Metal Oxides to Single Atoms in Carbon Nitrides

Jeppe V. Lauritsen

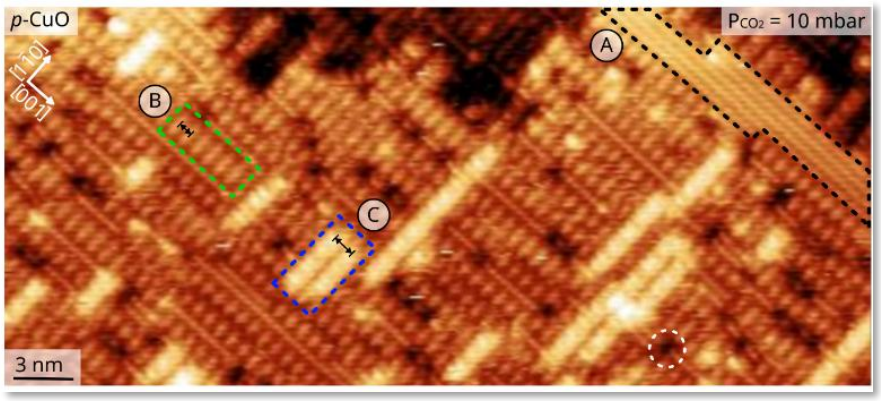
Interdisciplinary Nanoscience Center, Aarhus University, Denmark

*jvang@inano.au.dk

We pursue the goal of understanding fundamental properties of heterogeneous catalysts and electrocatalysts by focusing on what happens on the atomic level on surfaces. Surface science techniques, and in particular scanning probe microscopy methods, are excellent methods in this regard, since they allow us to image surfaces in atomic detail and characterize the interaction with reactants – even at elevated pressure conditions corresponding to catalytic conditions. I my talk I will discuss the advantages and limitations of applying scanning tunneling microscopy for investigation of planar models of technically relevant catalysts and electrocatalysts.

I will first give examples of how we use ambient-pressure scanning tunneling microscopy (AP-STM) to investigate atomic-details of reactive Cu surfaces, commonly used in catalysts for methanol production. Cu(110) is not reactive to CO_2 in vacuum conditions, but when the pressure is raised to several mbar, the surface structure converts, leading to a high Cu mobility and creation of a fascinating range of Cu-carbonate complexes. For CuZn/Cu(111), which is the active surface in industrial methanol synthesis, the response is quite different. Here the surface is stable in CO_2, but for CO containing gases at mbar pressure, Zn atoms are abstracted from the alloy, leading to a destabilization. The AP-STM work highlight how surface may dynamically respond to the gas composition they are exposed to [1,2].

In electrocatalysis studies, we have focused on single-atom catalysts reflecting highly dispersed metal species in a surface matrix, which are ideal for investigation by scanning probe microscopy methods. We have developed a planar model system that incorporates Co_1 single atom sites in a monolayer carbon-nitride on Au(111)[3]. Using an electrochemical cell seamlessly connected to the STM system, we can monitor the reactivity and investigate the characteristic structural changes and stability of resulting from contact to the electrochemical environment.



Near-ambient pressure (NAP)-STM image of partially oxidized Cu(110) in 10 mbar CO_2 [2]

References

[1] S. Jensen *et al.*, Nature Communications **15**, 3865 (2024).
[2] S. Jensen *et al.*, Angewandte Chemie International Edition **63**, e202405554 (2024).
[3] J. J. Gammelgaard *et al.*, ACS Nano **17**, 17489 (2023).

Formation of the surface alloy Au_2Sn driven by hydrogen etching of β-SnSe/Au(111)

S. Jiménez-Fernández [a], E. Tosi [a], V. Villalobos-Vilda [a], J.A. Martín Gago [a], José I. Martínez [a], C. Sánchez-Sánchez [a], I. Palacio [a]

[a] Instituto de Ciencia de Materiales de Madrid (ICMM-CSIC), Madrid, Spain

* sergio.j.f@csic.es

Bulk SnSe is a semiconducting material that stands out for its exceptional thermoelectric and optoelectronic properties along with its promising applications in photovoltaics. However, little less is known about its 2D form, β-SnSe, a metal monochalcogenide with a honeycomb structure that has been recently stabilized on Au (111) [1]. Atomic hydrogen plays an important role in the modification and transformation of surfaces at both the atomic and the macro scales. In this work, we report the room temperature transition of β-SnSe/Au(111) (Figure 1a) into Au_2Sn/Au(111) (Figure 1c), a surface alloy known for its Rashba state and potential spintronic applications [2], through a hydrogen-induced atomic modification, similar to that of Bi_2Se_3 [3]. The mechanism of such transformation is the following: Se gradually desorbs from the surface when β-SnSe is exposed to atomic hydrogen in the form of H_2Se. The remaining Sn atoms form the alloy with the Au atoms of the substrate, which migrate towards the topmost layer. Because of this migration, holes, whose size increases with the hydrogen exposure, appear (Figure 1b). This transformation has been studied by means of scanning tunneling microscopy (STM), low energy electron diffraction (LEED) and X-ray photoemission spectroscopy (XPS); and confirmed with ab-initio calculations.

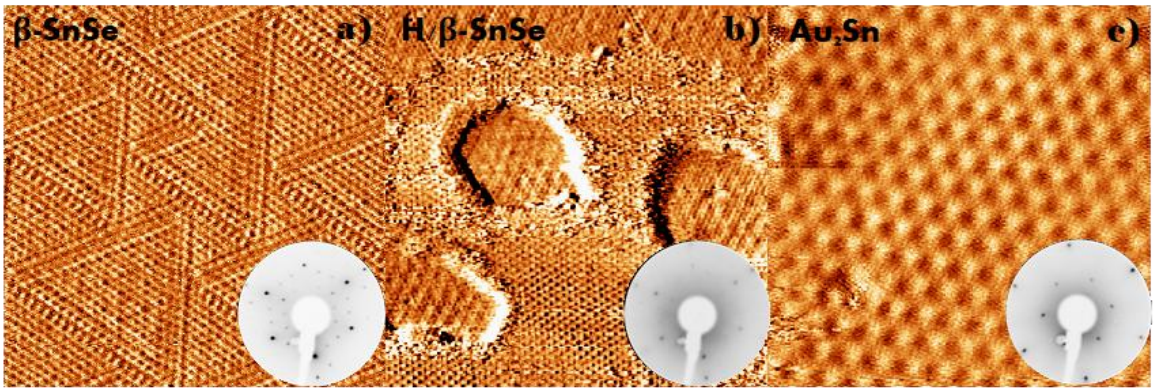


Figure 1. a) Current STM image of β-SnSe (Vb= 0.34 V; I= 0.43 nA; 15 x 15 nm2). b) Current STM image of H/β-SnSe (Vb= -0.73 V; I= 0.69 nA; 24.6 x 24.6 nm2). c) Current STM image of Au_2Sn (Vb= -1.8 V; I= 0.5 nA; 6 x 6 nm2). The insets show the LEED patterns acquired at E=80 eV.

References

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Electronic properties of Bismuth monolayers on metallic substrates

Kevin García Diez[1,2], J.Dai[2], J. E. Ortega[3,4,5], J. Lobo-Checa[6,7], M. Tallarida[2] and A. Mugarza[1,8]

[1]*Catalan Institute of Nanoscience and Nanotechnology (ICN2), CSIC and Barcelona Institute of Science and Technology, Campus UAB, Bellaterra, 08193 Barcelona, Spain*
[2]*ALBA Synchrotron Light Source, Carrer de la Llum 2-26, Cerdanyola del Vallès, 08290 Barcelona, Spain*
[3]*Donostia International Physics Centre, Manuel de Lardizabal 4, 20018-San Sebastian, Spain*
[4]*Centro de Física de Materiales CSIC/UPV-EHU, Manuel Lardizabal 5, 20018-San Sebastian, Spain*
[5]*Departamento de Física Aplicada I, Universidad del País Vasco, 20018-San Sebastian, Spain*
[6]*Instituto Ciencia de Materiales de Aragón, CSIC-Univ. de Zaragoza, E-50009 Zaragoza, Spain*
[7]*Dpto. Física de la Materia Condensada, Universidad de Zaragoza, E-50009 Zaragoza, Spain.*
[8]*ICREA Institució Catalana de Recerca i Estudis Avançats, 08010 Barcelona, Spain*
Kevin.garcia@icn2.cat

Bismuth, with its strong spin-orbit-coupling (SOC) and high carrier mobility, especially at its surfaces, has attracted considerable interest as spintronic and optoelectronic material. It is also an interesting case of topological material, with predicted high order topology [1]. At the monolayer limit, two different bismuthene allotropes have been grown (α and β), both showing topological edge states [2,3].

He we report a comprehensive study of the electronic and structural properties of Bi monolayers grown on Au(111) and Ag(111) substrates. Their atomic and electronic structure was investigated by Scanning Tunneling Microscopy and Spectroscopy (STM/STS), Low Energy Electron Diffraction (LEED), and Angle Resolved Photoemission Spectroscopy (ARPES). In both substrates, the monolayer follows a very similar (110)-like structure, with electronic structure dominated by the Moire pattern imposed by the substrate and Bi lattices. ARPES measurements reveal a profoundly perturbed electronic structure, affected by the Moire formed by the substrate and Bi layer, with strong coupling between the monolayers and the substrate, according to ab-initio calculations. When depositing alkali metals to intercalate and decouple the monolayers from the substrate, different surface reconstructions were found by LEED, corresponding ARPES measurements revealed modified band structures in all cases. Notably, Li/Bi/Ag(111) system is characterized by a hexagonal $\sqrt{3} \times \sqrt{3}$ LEED pattern and sharp, 2D hole-like bands. Both features are compatible with theoretical calculations for freestanding buckled β-Bismuthene available in the literature [4,5]. Our results indicate that alkali intercalation can be a useful strategy not only for electronic decoupling but also to stabilize structural phases that cannot be achieved otherwise.

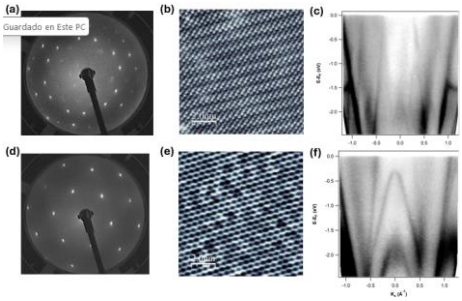

Figure 1: Respectively; LEED patterns, high-resolution STM images and band dispersion measured by ARPES for: (a)-(c) Bi(110) on Ag(111) and (d)-(f) Bi on Ag(111) after alkali intercalation.

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Unveiling the surface of model and realistic copper sulfides

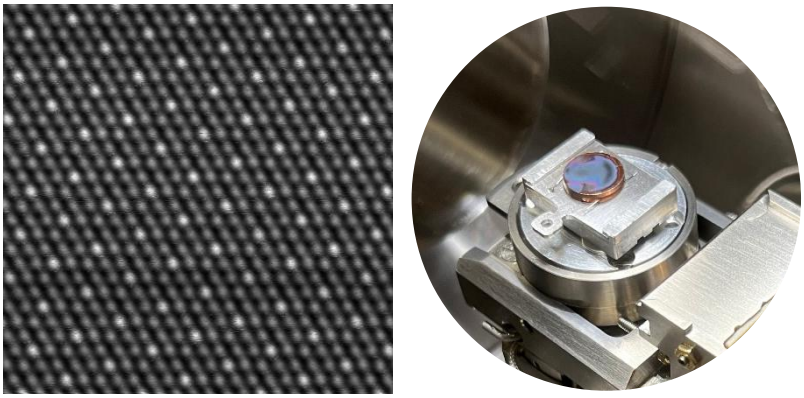
Roser Fernández-Climent [a], Aji Alexander [a], Pankaj Samal [a], Mateusz Wróbel [a], Josef Mysliveček[a], Martin Setvin, **Jesús Redondo** [a]*

[a] Department of Surface and Plasma Science, Charles University, Prague, Czech Republic

* jesus.redondo@mff.cuni.cz

Transition metal sulfides (TMS) are promising materials for electrochemical applications such as the hydrogen evolution reaction and the CO2 reduction reaction [1,2]. Contrary to oxides, TMS are mostly metallic or small band gap semiconductors, promoting efficient charge transport. Given a TM, there are plenty more stoichiometries and polymorphs of sulfides than oxides (e.g.: NiO vs NiS, NiS_2, Ni_3S_2, Ni_7S_6, Ni_3S_4), which offers a versatile toolbox for material scientists to tune the bulk and surface properties for a specific application [3]. Despite ready access to the macroscopic indicators of sulfide functionality in an electrochemical reaction (activity, selectivity, efficiency…), there is a vast lack of information about the fundamental properties that define said functionality (surface atomic and electronic structure, adsorption strength, vacancy formation…).

In this talk we explore the surface structure and chemistry of model and electrochemically-grown (realistic) copper sulfide surfaces. We cleave single crystals of CuS(0001) (Covellite) in UHV at different temperatures to expose model surfaces, Figure 1 left. Three distinct cleaved surfaces result from this method. We grow a realistic counterpart, Cu2S(111), on Cu(111) single crystals in a UHV-compatible electrochemical cell by open circuit potential and chronoamperometry techniques. The resulting film, Figure 1 right, is highly crystalline and clean and allows investigations by surface science tools. We investigate both materials by a combination of STM/nc-AFM, LEED, near-ambient pressure XPS and synchrotron-based XPS.



Copper sulfides – Left image: 10x10 nm^2 constant height STM image of a cleaving plane of CuS(00010. Right image: electrochemically-rown Cu_2S(111) film grown on Cu(111).

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Synthesis and characterization of a two-dimensional ionic hydride

A. Sáez-Coronado [a], D. Arribas [a], B. Cirera [a], J.I. Mendieta-Moreno [a], C. Gutiérrez-Cuesta [b], J.E. Prieto [b], J. De La Figuera [b], M. Garnica [c], I. Palacio [a], and P. Merino [a]

[a] *Instituto de Ciencia de Materiales de Madrid (ICMM-CSIC). c/ Sor Juana Inés de la Cruz 3, 28049, Spain*
[b] *Instituto de Química Física Blas Cabrera (IQF), CSIC, c/ Serrano 119, 28006, Madrid, Spain*
[c] *IMDEA Nanociencia, c/ Faraday 9, 28049, Madrid, Spain*

adrian.saez@csic.es

Hydrogen is a clean energy vector whose use is emerging strongly for a multitude of applications. However, its difficult storage hinders its potential as green fuel. So far, storage methods, such as high-pressure gas or liquid, do not meet energy density storage requirements or safety criteria, therefore, new storage methodologies are needed. An interesting alternative is the storage of hydrogen in solid materials such as hydrides. Ionic hydrides in its 3D form have been proposed and their hydrogen sorption kinetics characterized [1]. However, there is a lack of understanding of the properties of these materials under low dimensionality conditions down to the atomic scale [2]. In this work, we report the growth of a novel *hydrene*: a 2D layer of lithium hydride. The hydrogenation of a monolayer of lithium adatoms adsorbed on Au (111) leads to a honeycomb crystalline structure of lithium hydride. We have characterized LiH *hydrene* by means of scanning tunneling microscopy (STM), low energy electron microscopy/diffraction (LEEM/LEED), angle-resolved reflected-electron spectroscopy (ARRES), X-ray photoelectron spectroscopy (XPS) and density functional theory (DFT). The results confirm the formation of a bidimensional network of Li and H atoms arranged in a honeycomb structure. This new hydride structure opens the door to a new family of 2D materials made up of very light atoms and allowing a high gravimetric density [3].

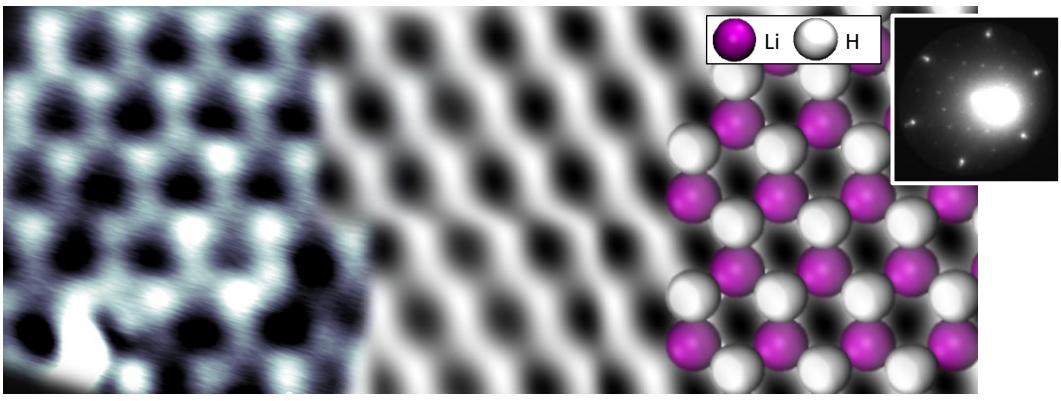

Figure 1. Experimental (left) and DFT best-fit simulation (centre) STM images (T = 77 K, I = 100 pA, V = -1.5 V) of the lithium hydride 2D network. Both images are merged in the central part. A schematic atomic model has been overlaid at right part. Inset: LEED pattern of the structure taken at 35 eV

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Unveiling the Origin of the Scale-Dependent Conductivity of Ni3(HITP)2 Metal-Organic Framework Thin Films

E. Osuna [a,b], P. Ares [a,b], J. Gómez-Herrero [a,b], G. Llauradó-Capdevila [c], D. Rodríguez-San-Miguel [d], S. Pané [e], J. Puigmartí-Luis [c,f], C. Gómez-Navarro [a,b]

[a] Departamento de Física de la Materia Condensada, Universidad Autónoma de Madrid, 28049 Madrid, Spain
[b] Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, 28049 Madrid, Spain
[c] Departament de Ciència dels Materials i Química Física, Institut de Química Teòrica i Computacional, Universitat de Barcelona, 08028 Barcelona, Spain
[d] Departamento de Química Inorgánica, Universidad Autónoma de Madrid, Madrid 28049, Spain
[e] Multi-Scale Robotics Lab (MSRL), Institute of Robotics and Intelligent Systems (IRIS), ETH Zurich, CH-8092 Zurich, Switzerland
[f] Institució Catalana de Recerca i Estudis Avançats (ICREA), 08010 Barcelona, Spain

* eva.osuna@uam.es

Conductive metal-organic frameworks (MOFs) are crystalline, intrinsically porous materials characterized by high electrical conductivity and exceptional structural and chemical versatility [1]. This rare combination of qualities makes these materials ideal for a wide range of energy-related applications [2]. However, the development of efficient MOF-based devices requires a thorough understanding of the charge transport mechanisms in conductive MOFs.

In this work, we conduct an in-depth study of the difference between nano- and micro-scale charge transport in $Ni_3(HITP)_2$ MOF thin films, which reveals that the conductivity in micron-sized MOF-based devices is mainly limited by crystallographic defects and poor electrical connections between grains in polycrystalline samples [3]. Our findings reveal a tenfold difference in conductivity between the micro- and nano-scale, attributed to poor electrical connections among a limited number of crystalline grains. We provide a value of the conductivity at the micro- ($\sigma_{IP,micro} = 0.7 \pm 0.3$ S/cm) and nano- ($\sigma_{IP,nano} = 7 \pm 3$ S/cm) scales, and find the value of the inter-grain resistance, $R_{inter\text{-}grain} = 40$ kΩ. We show that a resistor network model can reproduce our measured surface potential maps of in-operando MOF-based electrical devices. We also provide a structure-property relationship that links the density and spatial distribution of electrical failures in inter-grain connections of MOF thin films to their micro-scale conductivity.

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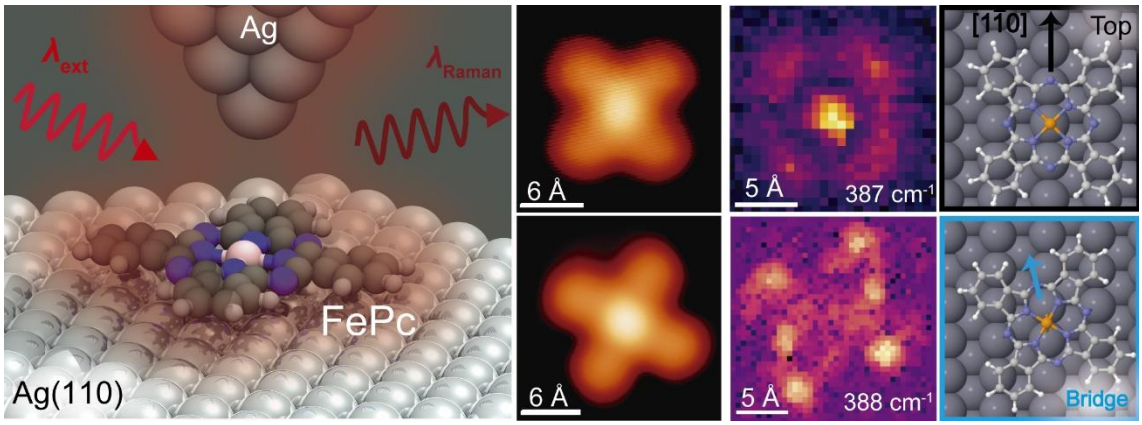
Atomic Precision Mapping of Site-Specific Vibrations in Single Molecules

Borja Cirera[1], Rodrigo Cezar de Campos Ferreira[2,3], Amandeep Sagwal[2], Jiří Doležal[3], Álvaro Gallego[4], Fernando Aguilar[4], Martin Švec[2,3], and Pablo Merino[1]

[1] Instituto de Ciencia de Materiales de Madrid, Spain
[2] Institute of Physics, Czech Academy of Sciences, Czech Republic
[3] Institute of Organic Chemistry and Biochemistry, Czech Academy of Sciences, Czech Republic
[4] Universidad Autónoma de Madrid, Spain

borja.cirera@csic.es

The vibrational landscape of adsorbed molecules is central to understanding surface interactions at the atomic scale, influencing phenomena ranging from catalysis to molecular electronics. Recent advances in atomic-scale tip-enhanced Raman spectroscopy (TERS) have enabled the vibrational mapping of single molecules by confining light in plasmonic picocavities [1], providing unprecedented insights into the heterogeneities of molecule-surface interactions with sub-nanometer resolution [2]. Here, we combine TERS, cryogenic scanning tunneling microscopy (STM) and density functional theory (DFT) calculations to explore Raman mapping of single iron phthalocyanine (FePc) monomers on three non-equivalent adsorption configurations on silver surfaces. We compare FePc molecules on Ag(111) and Ag(110), observing how subtle variations in adsorption geometry and registry with the underlying atomic lattice markedly influence molecular vibrational levels due to symmetry-induced modifications. Our results demonstrate the capabilities of TERS to map the site-specific vibrational properties of single molecules, providing direct evidence of how minor changes in the local atomic environment and the concomitant reduction of symmetry have a dramatic impact in the spatial distribution of vibrational levels. This work [3] not only establishes TERS mapping as a powerful technique across distinct surfaces to understand surface interactions, but also advances a novel tool for precisely tailoring chemical reactions at the atomic level.



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Light-matter interaction of field emission resonances in a scanning tunneling microscope

M. Varea[a,b], D. Mateos[b], K. Lauwaet[a],R. Miranda[a], R. Otero[a,b], A. Martín-Jiménez[a]

[a] *IMDEA Nanociencia, Madrid, Spain.*
[b] *Departamento de Física de la Materia Condensada, Universidad Autónoma de Madrid, Madrid, Spain.*

miguel.varea@imdea.org

The combination of scanning tunneling microscopy with laser light offers the unique possibility to investigate and control light-matter interaction at the atomic scale, which is critical for the development of novel technologies from diverse branches, such as quantum computing, optoelectronics, sensing, or catalysis, to mention a few. In our work, we investigate the effect of continuous wave (CW) laser illumination on the field emission resonances (FER) formed between a silver tip and a Ag(100) sample by measuring the derivative of the tunneling current as a function of the bias voltage. It was previously reported that the effect of CW illumination was that the lowest energy FER downshifts by the photon energy, being the hallmark of plasmon-assisted resonant tunneling [1]. We have extended these investigations and made a thorough experimental characterization of the effects induced by the laser power, tunneling current, and polarization of the excitation laser on the FERs. Interestingly, several peaks in the FER spectra appear/disappear upon laser illumination when varying polarization, laser power, or tunneling current, whose positions and intensities follow a non-trivial dependence (See Figure). Our observations cannot be described only assuming plasmon-assisted resonant tunneling, indicating that the strong field confinement of the laser fields due to the tip-sample nanocavity may be responsible for the observed effects.

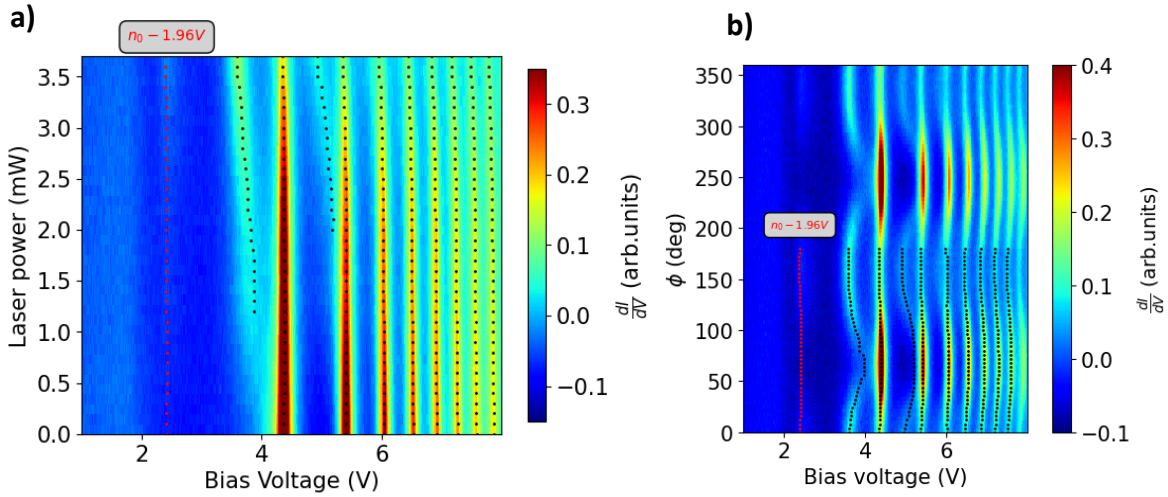

Figure – Color map of differential conductance spectra vs bias voltage for a series of laser power (a) and laser polarization direction (b) on Ag(100). The black dots follow the energy of the peak maxima for the FER peaks. The red points represent the energies of the n_0 peak minus the photon energy of the laser.

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Site-Specific Charge of a Ho atom on MgO

A. Pinar Solé [a,b], M. Ercelik [a,b], D. Borodin [a,b], J. Chae [a,b]
A. Heinrich [a,c]

[a] Center for Quantum Nanoscience (QNS), Institute for Basic Science (IBS)
[b] Ewha Womans University
[c] Department of Physics, Ewha Womans University

andrespinarsole@qns.science

We investigate the site-dependent relative charge of holmium (Ho) atoms adsorbed on MgO/Ag(100) [1] using Kelvin Probe Force Microscopy (KPFM) by means of a nc-AFM/STM qPlus sensor [2]. By manipulating a particular Ho atom between oxygen (Ho-O) and bridge (Ho-B) adsorption sites, we determine their relative charge via local contact potential difference (LCPD) measurements. KPFM parabolas reveal that Ho-O is positively charged, while Ho-B is negatively charged. Measurements at varying tip-sample distances show that atom-specificity is lost at far distances but is recovered at close approach, with significant charge variations between species. We also perform KPFM at constant height over the different absorption sites to spatially resolve the charge distribution along a particular direction. The results are analyzed in the context of electrostatic interactions, work function differences, and ab-initio modeling [3], providing insight into the absolute charge determination via KPFM height dependence.

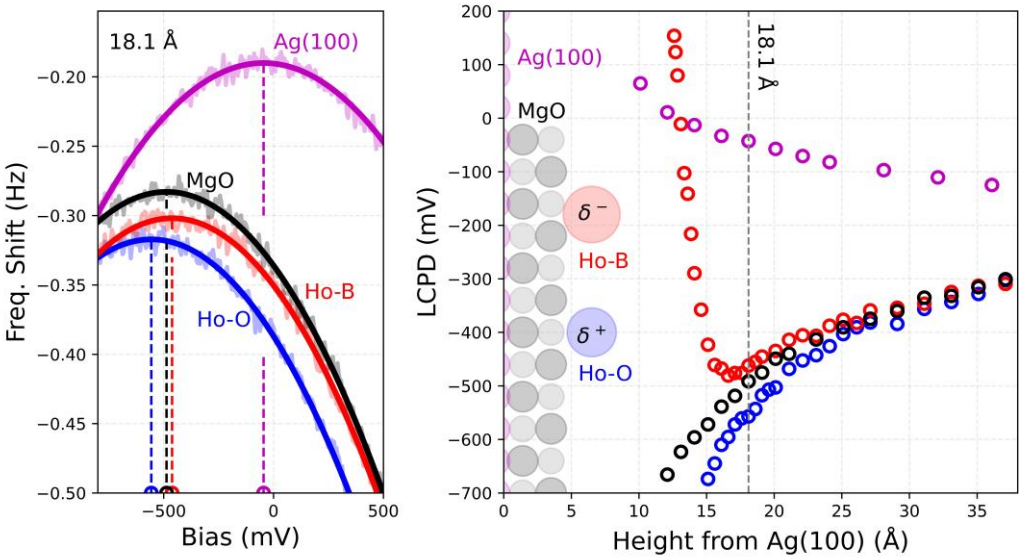

Figure – KPFM height dependence on different species

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Real-space imaging of π-holes

B. Mallada*[1,2,3+], M. Ondráček[1], M. Lamanec[3,4,5], A. Gallardo[1], A. Jiménez-Martín[1,2], B. de la Torre[1,2], P. Hobza[4,5], P. Jelínek[1,2]

[1] Institute of Physics, Czech Academy of Sciences, Prague, Czech Republic
[2] CATRIN, Palacký University Olomouc, Czech Republic
[3] Department of Physical Chemistry, Palacký University Olomouc, Czech Republic
[4] Institute of Organic Chemistry and Biochemistry, Czech Academy of Sciences, Prague, Czech Republic
[5] IT4Innovations, VŠB – Technical University of Ostrava, Czech Republic

* benjamin.mallada@bioch.ox.ac.uk

[+]Currently: Kavli Institute for Nanoscience Discovery, University of Oxford, Oxford, UK & Department of Biochemistry, University of Oxford, Oxford, UK

Non-covalent interactions driven by anisotropic charge distributions fundamentally govern molecular assembly, from DNA base-pair stacking to protein folding. Building on our real-space visualization of σ-holes[1], we now present the first direct observation of π-holes[2]- theoretically predicted electron-deficient regions perpendicular to aromatic planes.

Using Kelvin Probe Force Microscopy (KPFM), we achieve submolecular resolution of π-holes in halogenated anthracene molecules. Through comparative analysis with pristine anthracene, we reveal how π-holes influence the molecular ionization potential and determine molecular adsorption heights. The presence of π-holes significantly modulates stacking interactions between aromatic systems, a mechanism critical to biological processes such as nucleic acid stabilization and protein-ligand recognition. This work provides direct experimental evidence of π-holes and quantifies their role in molecular interactions, with implications for understanding biological structure stability and guiding rational drug design.

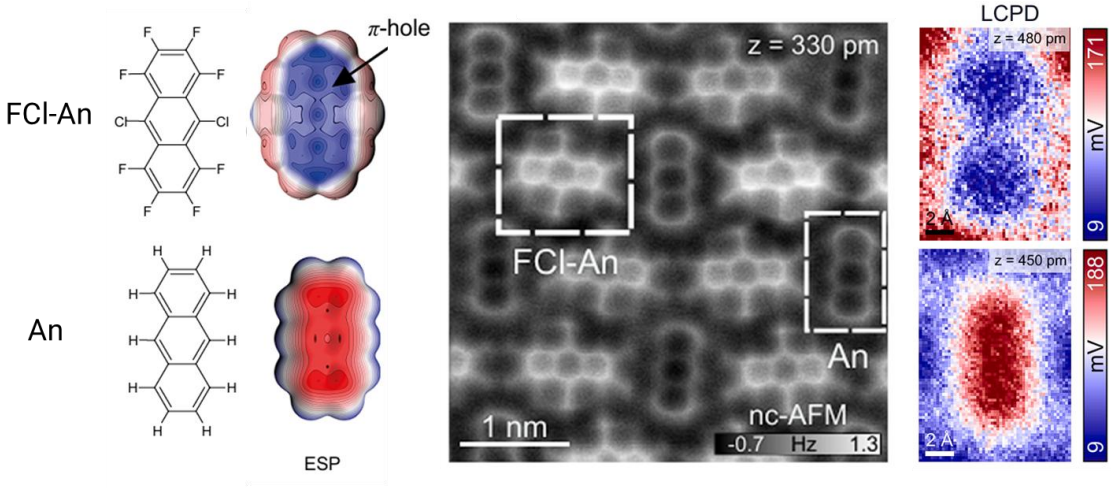

Figure – Model, ESP, ncAFM and KPFM measurements of halogenated and non-halogenated anthracenes.

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Open-shell character and charge-state control of an organic macrocycle on Au(111) and semiconducting $FeCl_2$

Oral contribution

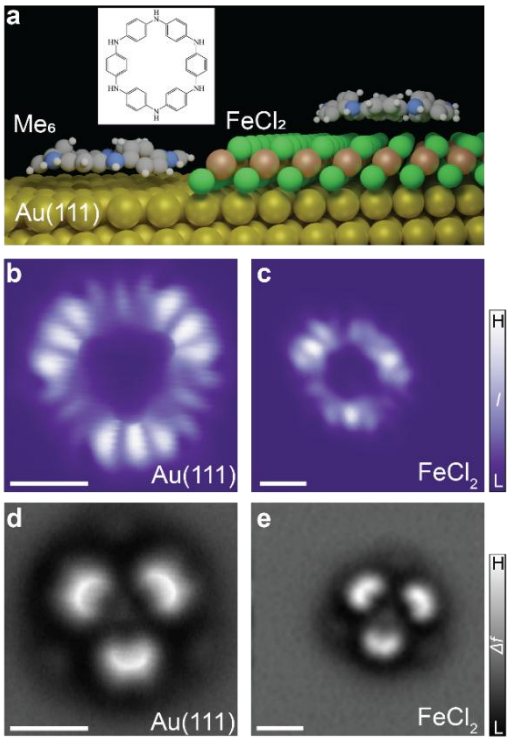
B. Lowe[a,*], O. Stetsovych[a], J. Berger[a], A. Pinar Sole[a], S. Louie[b], M. Lozano[a], M. Ondracek[a], P. Mutombo[a], S. Karmakar[a], D. Soler-Polo[a], M. Steigerwald[b], C. Nuckolls[b], P. Jelinek[a,*]

[a] Institute of Physics, Czech Academy of Sciences, Cukrovarnická 10, 162 00, Prague, Czech Republic

[b] Department of Chemistry, Columbia University, New York, New York 10027, United States

* lowe@fzu.cz; jelinekp@fzu.cz

Organic materials have emerged as attractive candidates for spintronics technologies given their tuneability. Though not traditionally considered magnetic materials, organic molecules can exhibit open-shell character on surfaces due to the stabilization of otherwise reactive products, and/or charge transfer between the molecules and the substrate. Here, we investigate individual macrocyclic emeraldine (Me_6) molecules on a metallic Au(111) surface, and on a semiconducting monolayer $FeCl_2$ surface[1] via scanning tunnelling microscopy (STM) and spectroscopy, non-contact atomic force microscopy (ncAFM), and Kelvin probe force microscopy supported by density functional theory calculations. We show that on Au(111), the molecular HOMO becomes singly occupied due to charge transfer resulting in an unpaired electron and hence a magnetic moment. This magnetic moment is Kondo screened by the metallic surface's conduction electrons. On $FeCl_2$, we demonstrate effective decoupling of the Me_6 molecules from the underlying metallic substrate as well as the ability to control the molecule's charge state via a double-barrier tunnel junction effect. This demonstration of control of the magnetic and electronic properties of an organic macrocycle highlights the importance of energy-level alignment in governing the properties of adsorbates.



a Illustration of Me_6 molecules (chemical structure in inset) on Au(111) and $FeCl_2$. **b-e** Simultaneously acquired constant-height STM (b,c) and ncAFM (d,e) images of individual Me_6 molecules on both surfaces. Scale bars: 5 Å.

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Nanoscale Electrostatics in Thin-Film Transistors: from Organic Semiconductors to 2D TMDs

Ana Pérez-Rodríguez [a], Daniel Vaquero [a], Daniel Martín-Jiménez [b], Juan Salvador-Sánchez [a], Inés Temiño [b], Marta Mas-Torrent [b], Vito Clericò [a], Esther Barrena [b], Carmen Ocal [b], Maha Labani [a], Enrique Diez [a], Jorge Quereda [c]

[a] Nanotechnology Group, USAL—Nanolab, Universidad de Salamanca, E-37008 Salamanca, Spain
[b] Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Campus de la UAB, Bellaterra, Barcelona 08193, Spain
[c] Instituto de Ciencia de Materiales de Madrid (ICMM-CSIC), Madrid E-28049, Spain

* perez.rodriguez.ana@usal.es

Kelvin probe force microscopy (KPFM) provides a powerful tool for visualizing local electrostatic potentials and characterize charge-transport mechanisms thin-film transistor (TFT) architectures. By performing in operando KPFM on functioning devices -applying gate and drain biases while tracking the resulting potential landscape- contact resistance and intrinsic channel effects can be characterized at nanoscale. In solution-processed organic TFTs based on organic electronic semiconductors fabricated via bottom-gate, top-contact geometries, KPFM reveals how crystalline domains and trap states limit carrier mobility. These insights guide improved device processing steps, such as controlling vertical phase separation or tuning electrode injection barrier for enhanced performance [1,2].
On the other hand, in few-layer thick flakes of ReS_2 -a distorted 1T-phase transition metal dichalcogenide with strong in-plane anisotropy- KPFM reveals electrostatic domains that remain uncorrelated with topography. Those electrostatic domains shift or invert under thermal treatment or applied bias, pointing out at interlayer sliding and possible ferroelectric-like behavior [3, 4]. By mapping local potential distributions in working ReS_2 TFTs, the intrinsic channel mobility can also be determined while separating out contact effects. Complementary low-energy electron microscopy (LEEM), ultraviolet photoemission electron microscopy (UVPEEM), and Raman spectroscopy help establish correlations between morphological and electrostatic changes.
These results highlight how KPFM helps connect crystal structure, electronic properties, and charge transport under real operating conditions, providing valuable insights for improving materials and device designs in both organic and 2D semiconductors.

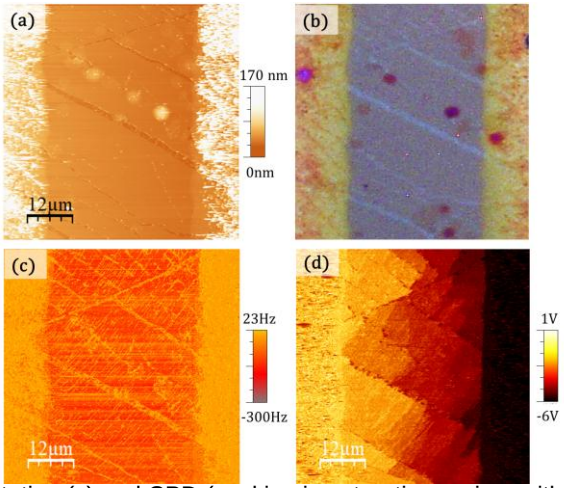

Figure - Topographic (a), excitation (c) and CPD (working in saturation regime with VGS= -6 V and VSD=-5 V) d) maps of the same channel area of C8-BTBT:PS TFTs. (b) Optical polarized microscopy images of the same area.

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Dielectrophoresis as a tool for investigating magnetic and transport properties of single magnetic nanowires by Magnetic Force Microscopy

E. Calle [a], A. Garcia-Martin [b], L. Álvaro-Gómez [c], L. Gómez-Cruz [c], J. Marqués-Marchán [d], L. Pérez [c, e], E. Burzurí [b], M. Jaafar [a]

[a] Instituto de Ciencia de Materiales de Madrid (ICMM-CSIC), Madrid, Spain
[b] Departamento de Física de la Materia Condensada and Condensed Matter Physics Center (IFIMAC), Facultad de Ciencias, Universidad Autónoma de Madrid, Madrid, Spain
[c] Departamento de Física de Materiales. Universidad Complutense de Madrid, Madrid, Spain,
[d] Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Straße 40, 01187 Dresden, Germany
[e] Instituto Madrileño de Estudios Avanzados en Nanociencia (IMDEA Nanociencia), Madrid, Spain,

* esther.calle@icmm.csic.es

Dielectrophoresis (DEP), the motion of of polarizable particles in a non-uniform electric field [1], has become a versatile tool for manipulating micro- and nanoscale objects across diverse fields, from industrial applications to biotechnology [2]. In this work, we use DEP to precisely control the motion of magnetic NWs to specific positions in a device [3], enabling the investigation of their magnetic and transport properties in-situ with scanning probe microscopies. Specifically, we have developed devices in which one or multiple nanowires can be easily positioned by means of the dielectrophoretic force generated by the application of a high-frequency AC electric field across micron-scale electrode gaps. This controlled placement is crucial for exploring individual nanowire properties, a frontier in 3D nanomagnetism [4,5]. Furthermore, we present a device including current paths perpendicular to the electrodes, designed as a proof-of-concept for studying the injection and manipulation of domain walls in individual nanowires using magnetic force microscopy (MFM) [6].

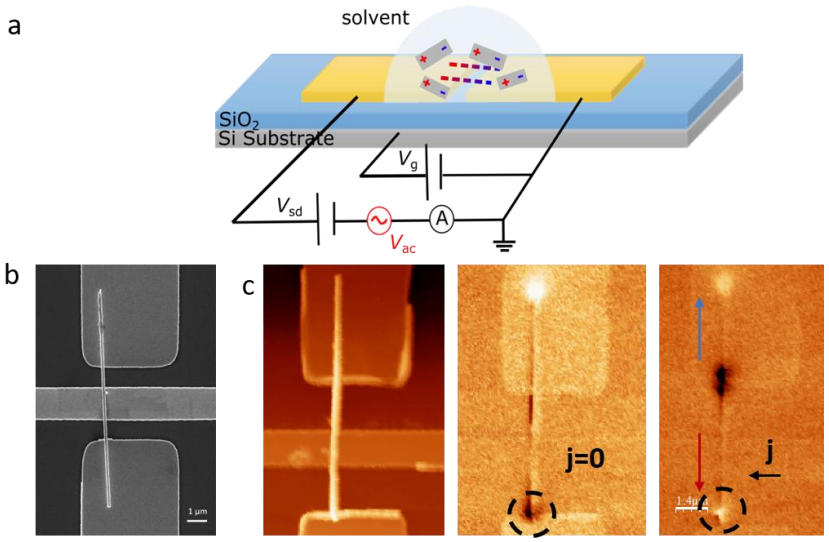

Figure (a) Schematic representation of the dielectrophoretic process (adapted from Martín Pérez, L. Doctoral thesis, 2024) (b) SEM image of a magnetic NW trapped by means of the dielectrophoretic force. (c) Topography and magnetic images of a single NW before and after applying a current pulse of 80 mA.

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Roughness induced magnetic domains changes in CoFeB/Pd multilayers

P. Martinez Outomuro[1]*, C. Belloso[1], C. García[2], G. López-Polín[3], D. Navas[1], A. Asenjo[1]

[1]*Instituto de Ciencia de Materiales de Madrid (ICMM-CSIC), 28049 Madrid, Spain.*
[2]*Universidad Técnica Federico Santa María, 2390123, Valparaíso, Chile*
[3]*Universidad Autónoma de Madrid, 20049, Madrid, Spain*
* pablo.martinez@csic.es

In a globalized world, where the demand for Internet of Things technologies continues to grow exponentially [1], reusing the waste heat they generate has become critical for reducing environmental impact. In this context, thermomagnetic generation through the Anomalous Nernst Effect (ANE) has been proposed as an alternative to the Seebeck Effect. While the latter exhibits high thermopower efficiency, the Nernst Effect, due to its transverse nature, enables the design of simpler generators as the thermal gradient and the generated electric field are perpendicular to each other [2].

Since the ANE voltage arises from the interplay of three different components through a tensorial product, having the magnetization in a well-defined direction is crucial for enhancing this effect [2]. For this purpose, we will grow magnetic multilayers of CoFeB/Pd, where perpendicular magnetic anisotropy (PMA) can be obtained [3]. In these multilayer systems, the interfacial roughness between the magnetic and non-magnetic material plays a key role in determining the thermomagnetic properties [2]. Our approach is to control the interface by adjusting the substrate roughness, using Si or SiN, which exhibit different roughness levels.

We have fabricated ultrathin [CoFeB (0.3nm)/Pd (1nm)]$_n$ samples, with different number of repetitions (n= 5, 10, 15). Given their strong PMA, the samples exhibit well-defined stripe domains (see MFM image in Figure 1). We have observed that slight variations in the macroscopic hysteresis loop measurements lead to noticeable changes in the local domain configuration. Moreover, the influence of the substrate-induced magnetic domain configuration on the ANE response will be determined.

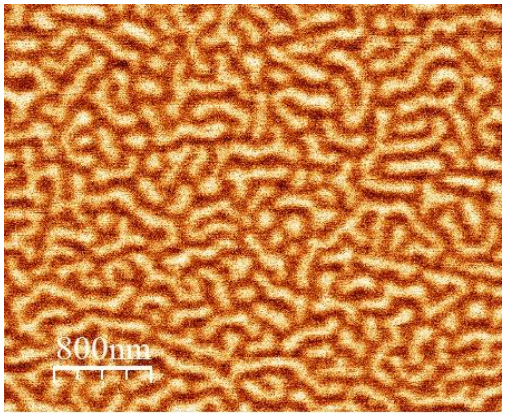

Figure 1: MFM image of the sample [CoFeB (0.3 nm)/Pd (1nm)]$_{15}$ grown onto SiN

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Customizing Magnetic Force Microscopy probes: going beyond standard imaging

J. Marqués-Marchán[a,b], M. Jaafar[a], E. M. Jefremovas[c,d], A. G. Gubieda[e], M. L. Fdez-Gubieda[f,g], M. Kläui[c], A. Asenjo[a]

[a] Instituto de Ciencia de Materiales de Madrid, CSIC, 28049 Madrid, Spain
[b] Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany
[c] Institute of Physics, Johannes Gutenberg University Mainz, 55128 Mainz, Germany
[d] Department of Physics and Materials Science, University of Luxembourg, L-1511 Luxembourg, Grand Duchy of Luxembourg
[e] Dpto. Inmunología, Microbiología y Parasitología, University of Basque Country (UPV/EHU), 48940 Leioa, Spain
[f] Dpto. Electricidad y Electrónica, University of Basque Country (UPV/EHU), 48940 Leioa, Spain
[g] BCMaterials, Basque Center for Materials, Applications and Nanostructures, UPV/EHU, Spain

* jorge.marchan@cpfs.mpg.de

Atomic force microscopy (AFM) is a powerful and accessible technique for the nanoscale characterization of different set of properties of materials such as structural, mechanical, chemical, or electrical properties. In particular, Magnetic Force Microscopy (MFM) has been widely used to explore the magnetic configuration of low-dimensional magnetic systems envisaged for different applications, as information technologies or energy harvesting [1].

Due to the broad use of the technique, commercial MFM probes with different properties (like high or low magnetic moment tips) are available and commonly used by the users. However, this catalogue is limited and not enough when characterizing some materials, since with these probes the tip may modify the magnetic configuration of the sample, leading to artifacts, or the magnetic signal is too low to be detected. Consequently, a step forward standard MFM and probe engineering is required in such cases.

In this work, we present strategies to obtain the suitable magnetic probes by tailoring their mechanical and/or magnetic properties, as well as their performance in challenging materials. For example, magnetic nanorods grown on mechanically soft cantilevers enable the detection of magnetic features in biological samples (see Figure), opening the path to the use of MFM in the life science field [2]. Also, in a different approach, ultralow moment magnetic tips enable the visualization and manipulation of the magnetic textures in magnetic multilayers [3,4], not possible with the commercially available standard nor low moment tips. These results pave the way for the proper design of probes and continued use of MFM to investigate a vast range of new materials.

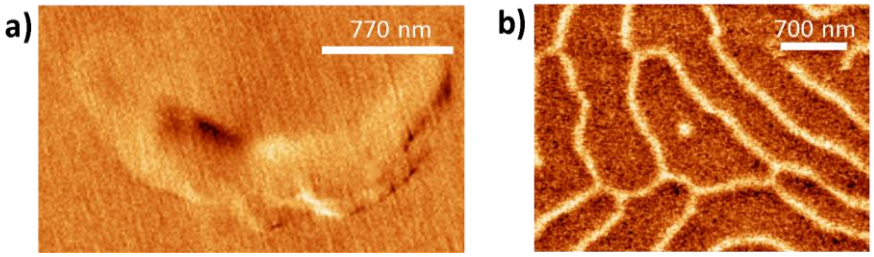

Figure – MFM images acquired with customized probes of (a) a *Magnetosprillum gryphiswaldense* bacterium [2], and (b) magnetic multilayer stack [3].

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Magnetic field screening of 2D materials revealed by magnetic force microscopy

D. A. Aldave[a], G. López-Polín[b], E. Calle[a], A. Begué[c,d], R. Ranchal[c], R. Martínez[e], C. Bran[f], E. Burzurí[a], J. Gómez-Herrero[a], P. Ares[a], M, Jaafar[e]

[a] Department of Condensed Matter Physics and Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, 28049, Madrid, Spain
[b] Department of Physics of Materials, Universidad Autónoma de Madrid, 28049, Madrid, Spain
[c] Department of Physics of Materials, Universidad Complutense de Madrid, 28040, Madrid, Spain
[d] Faculty of Science, Universidad de Zaragoza, 50009, Zaragoza, Spain
[e] Instituto de Ciencia de Materiales de Madrid (ICMM) and Consejo Superior de Investigaciones Científicas (CSIC), 28049, Madrid, Spain
[f] Instituto de Nanociencia y Materiales de Aragón (INMA-CSIC), Universidad de Zaragoza, 50009, Zaragoza, Spain

* diego.aldave@uam.es

Two-dimensional (2D) materials possess exceptional mechanical properties, making them promising candidates for protecting nanostructures. However, the magnetic field screening properties of 2D materials are largely unexplored.[1] Here, Magnetic Force Microscopy (MFM) is used to unveil the effects on the magnetic field of magnetic nanostructures when 2D materials are placed on top of them. It is demonstrated that while graphene and few layer graphene (FLG) exhibits a weak diamagnetic response due to its unique electronic structure around the Dirac point, the overall screening effect remains minimal (~0.5% per layer). Conversely, graphene oxide (GO) and MoS_2 show negligible response to the magnetic field, making them ideal for applications where preserving the original magnetic properties is crucial. These findings suggest that 2D materials can offer effective protection while minimally affecting the underlying magnetic functionalities, important for data storage technologies and spintronics.

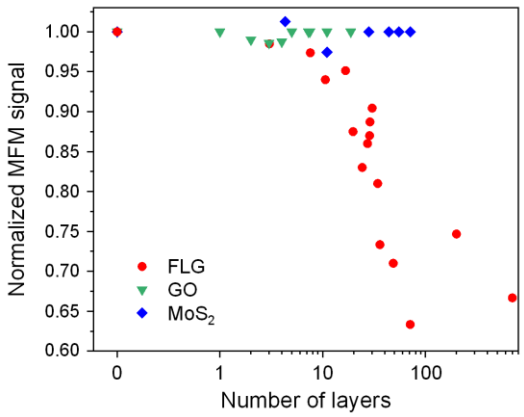

Figure - Magnetic field screening quantified by the decrease of the MFM signal for regions covered by FLG, GO,

and MoS2 as a function of the number of layers.

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Porphyrin-GO nanohybrids: insights into morphological, optical, and electronic properties at the nanoscale

M. Navarro-Rodríguez[a*], V. Camús[b], A. Cros[b], N. Garro[b], E. Palacios-Lidón[a]

[a] Universidad de Murcia, Centro de Investigación en Optica y Nanofisica (CIOyN), Murcia, 30100, Murcia, Spain

[b] Universitat de València, Institut de Ciència dels Materials (ICMUV), Paterna, 46980, València, Spain

* mario.navarror@um.es

Functionalized graphene oxide (GO) and reduced graphene oxide (RGO) hybridized with dye molecules, particularly porphyrins, have emerged as promising platforms due to their unique photoactive properties. Porphyrins, owing to their natural abundance and excellent spectroscopic and electrochemical characteristics, offer great potential for applications in optoelectronics, sensing, photocatalysis, and medical therapies. Despite significant experimental advancements, a deeper understanding of the structural, electronic, and optical interactions within these nanohybrids, particularly in solid-state devices, remains crucial.

In this work, we investigate the non-covalent hybrids of GO and RGO with protoporphyrin IX (PPIX) using co-localized Kelvin Probe Force Microscopy, photoluminescence (PL), and Raman spectroscopy. These techniques provide nanoscale insights into the morphological (Fig. 1a), b)), electronic, and optical properties of individual flakes, enabling the monitoring of light-induced processes at the dye/graphene-derived material interface. Our results reveal that molecular aggregation and charge transfer processes differ significantly between GO and RGO, leading to distinct fluorescence behaviors. Specifically, the porphyrin/GO hybrid exhibits enhanced fluorescence, whereas fluorescence quenching is observed in the porphyrin/RGO system (Fig. 1c)). Furthermore, local surface photovoltage measurements reveal charge transfer processes in the rGO/PPIX hybrids (Fig. 1d), e)), providing an explanation for the fluorescence quenching observed in the system.

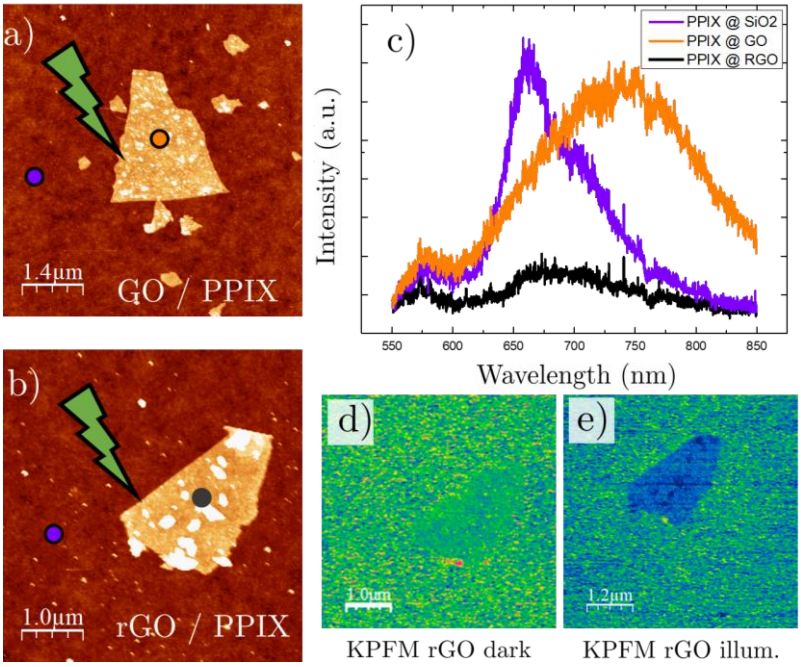


Figure – Topography of the a) GO-PPIX hybrids, b) RGO-PPIX hybrids. Z scale 10 nm. c) PL spectra obtained on GO, RGO and SiO_2. KPFM images of the d) RGO-PPIX hybrid under dark, and e) under illumination. Z scale 100 mV

A versatile technological UHV-compatible AFM: adhesion and friction mapping in Ultra High Vacuum

D. Gallego-Fuente [a,b,*], P. Ares [a,b], J. Gomez-Herrero [a,b]

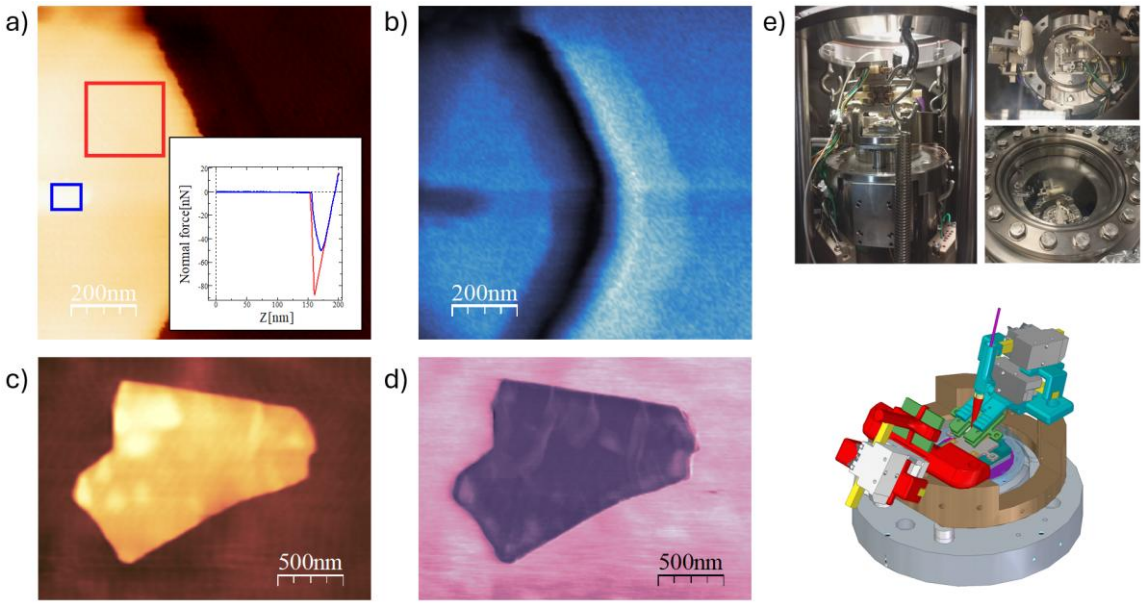
[a] Departamento de Física de la Materia Condensada, Universidad Autónoma de Madrid, Spain
[b] Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, Spain

* daniel.gallego@uam.es

Atomic Force Microscopy (AFM) has undergone continuous advancements, enabling increasingly specialized measurement approaches across a broad range of applications.

Building upon these previous advances, a novel technological AFM system has been developed for operation in Ultra High Vacuum (UHV) at room temperature, combining the versatility of standard AFMs with the capabilities required for UHV environments. Unlike conventional UHV AFMs, which are optimized for atomic-scale resolution but lack broader functionality, this system integrates advanced measurement modes, sample manipulation, lithography and optical sample localization. It can alternate between two distinct XYZ scanners optimized for either short- or long-range scanning, in combination with a beam deflection method for both normal and lateral force detection, allowing adhesion[1] and friction[2] studies in UHV.

As a demonstration of its capabilities, adhesion and friction mapping of samples in UHV has been performed. This result highlights the instrument's potential for nanoscale characterization, extending the capabilities of the laboratory to experiments in the most controlled environment.



a) Topography and b) adhesion images obtained in UHV of a mechanically exfoliated MoS_2 flake. Inlet: average adhesion curve for marked regions c) Topography and d) lateral force images obtained in UHV of a mechanically exfoliated MoS_2 flake. e) Images and diagram of the AFM head enclosed in the UHV chamber

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Tautomerization processes and molecular defects revealed by scanning probe microscopy and first-principles calculations

Carlos Romero-Muñiz*[a], Pablo Pou[b], Rubén Pérez[b]

[a] Departamento de Física de la Materia Condensada,
Universidad de Sevilla, PO Box 1065, 41080 Sevilla, Spain
[b] Departamento de Física Teórica de la Materia Condensada and Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, E-28049 Madrid, Spain

* crmuniz@us.es

Scanning Tunneling and Atomic Force microscopies are nowadays essential techniques to characterize and manipulate molecules adsorbed on surfaces. This is due to their capability of resolving the internal structure of molecular, including their main submolecular features. Moreover, on-surface chemical reactions can be tracked, controlled or induced by scanning probe tips. However, the use of theoretical models has become essential to achieve a proper understanding of the experimental results, often difficult to rationalize [1,2].

In this work, we show, in two different contexts, how the combination of high-resolution scanning probe microscopy at low temperatures and first-principles calculations based on density functional theory is a powerful tool for the study of molecular systems deposited on surfaces. On the one hand, we study the adsorption of *meso*-dibenzoporphycene molecules –a constitutional isomer of porphyrin— on Ag(111) and on 2-monolayer-thick NaCl films [3]. In particular, we focus on tautomerization processes (i.e., when hydrogen atoms are transferred within the molecule) and we demonstrate how the molecule-substrate interaction plays a major role in the stability and imaging of these tautomers, which cannot be isolated in gas-phase or dissolution. On the other hand, we use a similar approach to gain fundamental insight into the behavior molecular islands of CO_2 grown on Au(111) [4]. Challenging the common view, we demonstrate that weakly physisorbed CO_2 molecules on this substrate form self-assembled islands instead of periodic monolayers, showing a distinctive windmill-like structure that encloses a standing-up CO_2 molecule and a number of unusual defects (see figure). We identify the species responsible for these defects, clarifying the origin of the kagome tiling exhibited by this surface system.

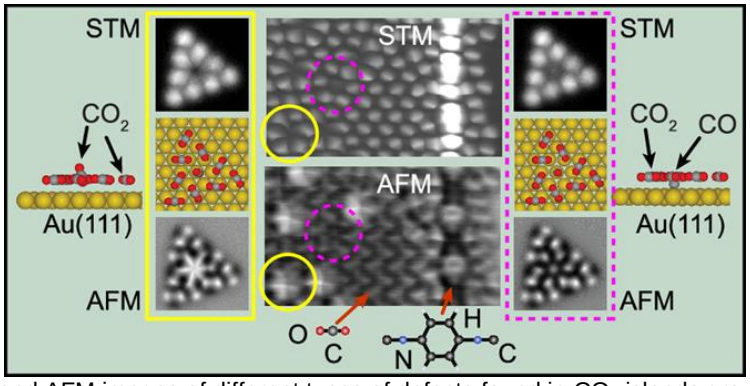

Figure – STM and AFM images of different types of defects found in CO_2 islands grown on Au(111).

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Computational characterization of low-dimensional molecular nanostructures and their SPM imaging.

Aurelio Gallardo [a] Elena Pérez-Elvira[a], Ana Barragan[a], Jonas Björk[b], José I. Urgel[a], David Écija[a]

[a] IMDEA Nanociencia, C/ Faraday 9, Campus de Cantoblanco, Madrid, 28049
[a] Linköping University, SE-581 83 Linköping, Sweden

* aurelio.gallardo@imdea.org

On-surface chemistry represents a fast-growing field that enables the synthesis of molecular structures that are not accessible through traditional wet chemistry. In this context, high-resolution scanning probe microscopy (SPM) techniques provide unprecedented spatial resolution, allowing for the precise identification of individual reaction products. Nevertheless, a deep understanding of the reaction mechanisms under the conditions imposed by the substrate remains elusive.

To address this, various computational strategies are available to characterize the optimal reaction pathways of chemical processes occurring on solid surfaces and to analyze reaction stages using SPM techniques. For example, molecular dynamics (MD) methods within the canonical ensemble, based on the QM/MM (quantum mechanics/molecular mechanics) description of interatomic forces, allow for the simulation of very large systems at a relatively low computational cost. On the other hand, SPM approaches such as the Probe particle model [1] had demonstrated mighty potential for the simulation of AFM, IETS, STM and KPFM experiments.

In this presentation, I will discuss the experimental and computational results of various projects in which we employ these computational approaches to gain a better understanding of on-surface synthesis experiments conducted by our group. Examples include (i) the stepwise transformation of coronene-based organometallic networks into two-dimensional covalent patches (see Figure 1a) [2], and (ii) the Co-metalation of Hemiporphyrazine macrocycles (see Figure 1b) [3].

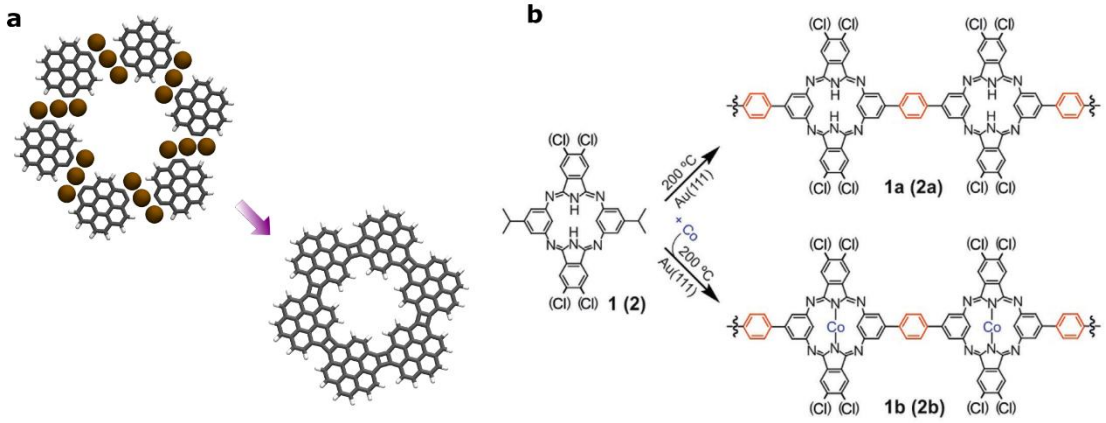

Figure 1. Schematic description of a) the transformation of coronene-based organometallic networks into two-dimensional covalent patches, b) the on-surface formation of indenyl based polymers

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Accurate forces for CO tips on cobalt phthalocyanines on Ag(111)

J. Trujillo-Mulero[a], X. Wang[b], E. Ventura-Macias[a], E. Altman[b], P. Zahl[c], U. Schwarz[b], R. Pérez[a]

[a] Departamento de Física Teórica de la Materia Condensada & Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, E-28049, Madrid (Spain)
[b] Department of Mechanical Engineering and Materials Science & Department of Chemical and Environmental Engineering, Yale University, New Haven, Connecticut 06511 (USA)
[d] Center for Functional Nanomaterials, Brookhaven National Lab, Upton, New York 11973 (USA) States)

* jara.trujillo@uam.es

Recent studies have revealed that cobalt phthalocyanines (CoPcs) immobilized on carbon nanotubes, a hybrid catalyst, enhance methanol production from CO_2 [1]. In particular, the interaction strength between the intermediate CO and the central Co atom is a critical factor influencing catalytic performance. To explore the subtle characteristics of this interaction, Wang et al. [2] have used a novel 3D scanning methodology with a high-resolution atomic force microscope (HRAFM) with a CO-functionalized tip to study CoPc molecules on Ag(111) at the single-molecule level. Here, we validate this extensive experimental study with density functional theory (DFT) and the full-density-based model (FDBM) [3,4] for HRAFM. Our DFT simulations reveal that the most stable adsorption configuration for a CoPc molecule on Ag(111) is the cobalt metal atom on a bridge site with one of the wings aligned with the silver's close-packed direction, as seen in Fig. 1 a). Then, using the FDBM, we confirmed Wang et al.'s method for isolating CO tip-sample interactions from substrate and metallic tip effects. The differences between the experimental and theoretical force curves indicated the molecule was being bent by effect of the CO tip. Taking into account the stiffness of the molecule, the curves show a remarkable agreement, Fig 1. d) [5]. We extended this study to $CoPc(NH_2)_4$ (Fig. 1 second row) and compared the electronic structure of both molecules, analyzing the effect of the amino groups. Finally, we have looked for possible explanations to the unusual spot that appears quite frequently associated to $CoPc(NH_2)_4$ (lower left corner of the experimental image in Fig. 1 h).

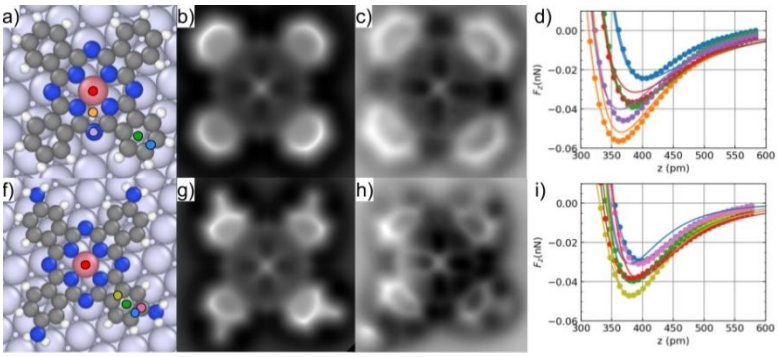

Figure 1 – Most stable configuration for a CoPc (first row) and $CoPc(NH_2)_4$ (second row) molecules absorbed on a Ag(111) surface (a, f) and AFM frequency shift images: simulated (b, g) at 346pm of the tip-sample separation and experimental (c, h) at 65pm (CoPc) and 30pm ($CoPc(NH_2)_4$) from the point of closest approach [3]. d) and i): force curves for the experiment (line) and our FDBM theoretical model (circles)

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Revisiting the formation of water nanomenisci

O. Mateos-Lopez[1,2], J. G. Vilhena[2], and J. C. Cuevas[1,3]

[1]Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, E-28049 Madrid, Spain

[2]Instituto de Ciencia de Materiales de Madrid, CSIC, c/Sor Juana Ines de la Cruz 3, 28049 Madrid, Spain

[3]Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, E-28049 Madrid, Spain

* oscar.mateosl@uam.com

Under normal conditions, the presence of a Scanning Probe Microscope tip at nanometers from a surface is known to favor the condensation of water molecules from the air into a meniscus, connecting tip and surface. The shape and size of this meniscus depends on the tip shape and the local humidity, in accordance with the Kelvin Equation, whose validity has been confirmed at the nanoscale [1,2]. According to these studies, under high-vacuum conditions the local humidity would be defined as near-zero, and therefore a water meniscus should not exist. However, recent experiments [3] indicate that water menisci do exist even under these conditions. In our work, we make use of Molecular Dynamics (MD) to show that this is possible because the water molecules condensing into the meniscus come from the water chemisorbed on the surface, see Fig. 1. Using a combination of MD simulations and existent macroscopic models, we are able to characterize the formation, size, shape, capillary forces and thermal conductance of these nanoscopic water structures.

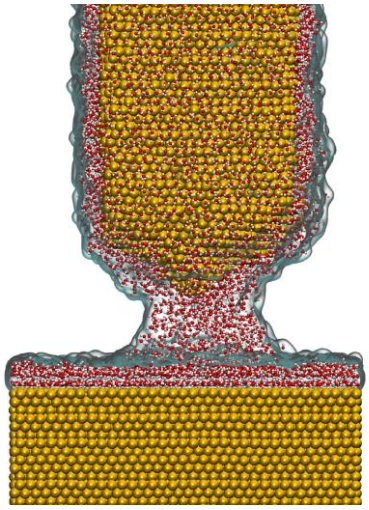

Figure 1 - Atomic representation of our system. Our contacts are a gold surface and a gold tip. A water neck formed from adsorbed water connects them.

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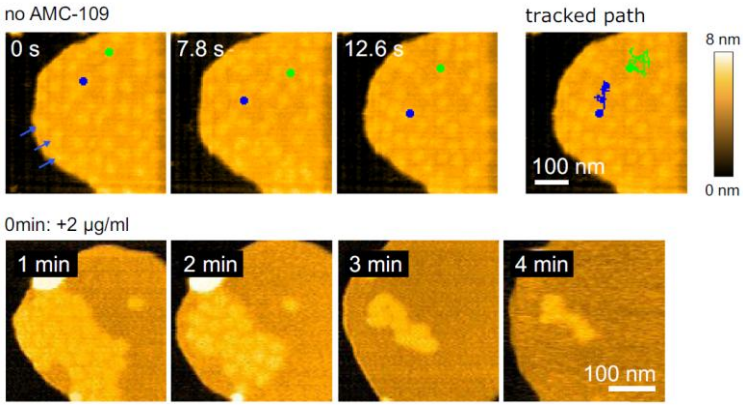
Nanoscale dynamics of biomolecular interactions: from viruses to antibiotics

Wouter H. Roos

Moleculaire Biofysica, Zernike Instituut, Rijksuniversiteit Groningen, the Netherlands

E-mail: w.h.roos@rug.nl

Using (High Speed) Atomic Force Microscopy and supporting single molecule approaches we scrutinize the stability and dynamics of supramolecular assemblies at the nanoscale, in real time. I will show how we are using these techniques to unveil the fascinating world of sub-cellular mechanics and biomimetic assembly processes. This will be illustrated by discussing the stability of single viral and virus-like particles and scrutinizing the relation between mechanics and infectivity. Next assembly and disassembly of protein complexes and its dynamic visualization will be discussed. Furthermore, real-time studies of the self-assembly of virus-like-particles (VLPs) are shown, revealing dynamic binding of capsid proteins to dsDNA and the appearance of stable VLP structures around the genome. The formation dynamics of 2D capsid protein assemblies is analysed, particularly showing how complex the kinetics of viral self-assembly can be, with multiple assembly pathways and continuously occurring assembly and disassembly events. Finally the mode of action of antibiotics is discussed and examples are given of how we can scrutinize the dynamic attachment of antibiotic compounds to membranes and the subsequent remodelling of the membrane (see figure).



Mode of action of the antibiotic AMC-109: The antibiotic

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Through the Lens of Force: Deciphering Melbournevirus' Structural Secrets through Atomic Force Microscopy

Alejandro Díez-Martínez [a], Adrián Cámara [a], Audrey Lartigue [b], Chantal Abergel [b], Pedro J. de Pablo [a]

[a] Departamento de Física de la Materia Condensada, Universidad Autónoma de Madrid, Spain
[b] Information Génomique & Structurale, UMR7256, Aix-Marseille University, Centre National de la Recherche Scientifique, France

* alejandro.diez@uam.es

Since the discovery of the first giant virus in 2003 [1], interest in this type of virus has only grown. Their infection cycle is based on phagocytosis by a host, in most cases amoebas. However, many morphological peculiarities of these now numerous families remain unknown [2].

Here, we focus on melbournevirus, a member of the family *Marseilleviridae*, which was discovered in a freshwater pond in Australia in 2014 [3]. Its capsid diameter ranges from 190 to 250 nm with a double-layered membrane and a dsDNA. However, many questions about this virus remain unanswered. Cryo-EM images have consistently revealed a large and dense body (LDB) in all samples examined, although its function is still unknown [4]. In addition, the possible clustering of histones into nucleosome-like particles has been investigated, but direct visual evidence is still lacking [5,6].

In this study, we used atomic force microscopy (AFM) to investigate both the internal contents of melbournevirus and the unusual physicochemical resistance of its structure. To achieve this, we subjected the virus to various mechanical stresses, urea treatments, pH variations, detergents, and drying tests, providing new insights into the properties of this remarkable virus.

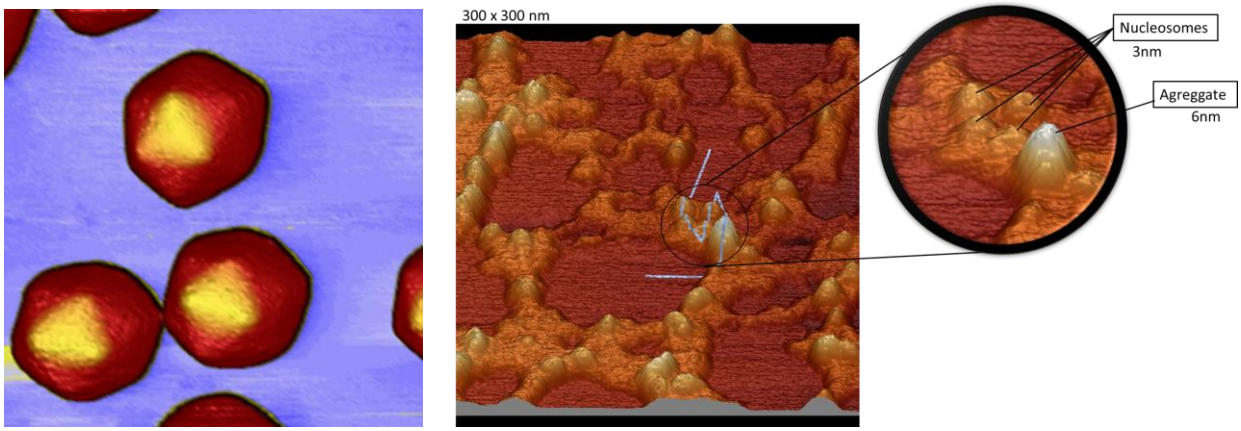

Figure 1. Left: AFM image of melbournevirus (1 µm x 1 µm). Right: 3D AFM image of melbournevirus genome.

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Structural Characterization of RNA combining AFM, Chemical Probing and Dynamic Fitting

E. M. Martín-Cuevas*[a], C. Aicart-Ramos[a], Salvatore Assenza[b] and F. Moreno-Herrero[a]

[a] *Department of Macromolecular Structures, Spanish National Center of Biotechnology (CNB), Spanish National Research Council (CSIC), 28049, Madrid, Spain*
[b] *Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, E-28049 Madrid, Spain*

* em.martin@cnb.csic.com

The secondary and tertiary structures adopted by single-stranded RNA molecules play a crucial role in determining their function in cellular processes. However, the majority of RNAs remain structurally uncharacterized, and the relationship between nucleotide sequence and final folded conformation is not yet fully understood. In this study, we employ Atomic Force Microscopy (AFM) to investigate RNA secondary structure and conformational dynamics, as it enables direct visualization of structural heterogeneity at the single-molecule level. Moreover, we integrate AFM imaging with advanced image analysis and Molecular Dynamic simulations to gain insights into the secondary structure of RNAs. We apply a dynamic fitting approach based on [1][2], leveraging coarse-grained molecular dynamics simulations to validate chemical-probing-derived secondary structures against AFM experimental images.

As a proof of concept, we apply this methodology to the 5′ proximal region of SARS-CoV-2, demonstrating its ability to resolve structural features and conformational flexibility (Figure 1). We further extend this approach to longer RNAs with more complex architectures, incorporating modifications such as 5′ and 3′ tagging with poly-A tails and targeted oligonucleotide-induced structural disruption. Our work underscores the advantages of AFM in capturing global RNA conformations, which, when combined with high-resolution techniques such as chemical probing, can provide deeper insights into RNA structural organization and function.

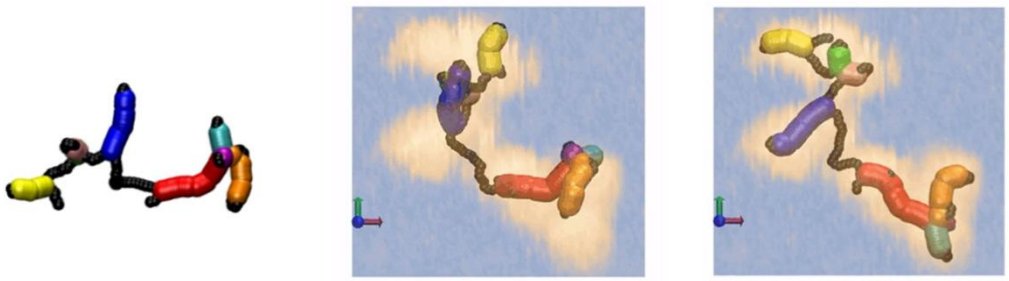

Figure 1 – Dynamic Fitting of the 5' proximal region of Sars-CoV-2. Coarse-grained model obtained from published Secondary Structure [3]

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Highthroughput Biomechanical Characterization of Macrophage Polarization Through Atomic Force Microscopy

Beatriz Cantero Nieto [a], Annalisa Calò [a,b], Gabriel Gomila Lluch [a,b], Mauricio Cano Galván [a]

[a] Institute for Bioengineering of Catalonia, Carrer Baldiri Reixac 10-12, 08028 Barcelona (Spain)
[b] Physics Faculty, University of Barcelona (UB), Carrer de Martí i Franquès 1-10, 08028 Barcelona (Spain)

bcantero@ibec.barcelona.eu

Macrophages play a critical role in innate immunity and are involved in a wide range of biological functions. Due to high plasticity, macrophages can be polarized into different phenotypes depending on the microenvironment, enabling them to perform specific functions during inflammation. This polarization capability underscores the importance of identifying biomechanical differences between various macrophage subtypes, as these variations could serve as valuable indicators for early diagnosis in various diseases Including chronic inflammatory diseases (such as rheumatoid arthritis, fibrosis, and atherosclerosis), neurodegenerative diseases, and cancer [1].

However, neither standardized measurement protocol or robust biomechanical analysis currently exists to efficiently explore these differences. In this context, atomic force microscopy (AFM) has emerged as an ideal tool, as it allows mapping cellular biomechanical properties with high spatial resolution under physiological conditions. To enable precise identification and differentiation of these phenotypes, we present a measurement protocol in which key experimental parameters are carefully controlled, along with the development of accurate analytical models and advanced data analysis techniques integrated with artificial intelligence. These results open new avenues for macrophage research and, more broadly, for highthroughput cell nanomechanical studies, projecting the AFM technique into real clinical applications.

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Atomically resolved imaging of the conformations and adsorption geometries of individual β-cyclodextrins with non-contact AFM

M. Grabarics[a,b], B. Mallada[c,d], S. Edalatmanesh[c,d], A. Jiménez-Martín[c,d], M. Pykal[d], M. Ondráček[c], P. Kührová[d], W. B. Struwe[b], P. Banáš[d], S. Rauschenbach[a,b], P. Jelínek[c,d], B. de la Torre[c,d,e]

[a] Department of Chemistry, University of Oxford, OX1 3QU Oxford, UK
[b] Kavli Institute for Nanoscience Discovery, University of Oxford, OX1 3QU Oxford, UK
[c] Institute of Physics, Czech Academy of Sciences, 16200 Prague, Czech Republic
[d] CATRIN, Palacký University Olomouc, 78371 Olomouc, Czech Republic
[e] Nanomaterials and Nanotechnology Research Center, CSIC-UNIOVI-PA, 33940 El Entrego, Spain

* grabaricsmarko@gmail.com

Glycans, consisting of covalently linked sugar units, are a major class of biopolymers that are essential to all known living organisms. To better understand their various biological functions, resolving the structure of glycans is of key importance. The size, complexity, flexibility, and heterogeneity of these molecules, however, often makes their analysis challenging using traditional spectroscopic and diffraction methods, which require many molecules to be probed simultaneously and thus provide only ensemble-averaged information.

Here, we combine electrospray deposition in ultra-high vacuum with non-contact AFM and first-principles calculations to unravel the structure of β-cyclodextrin, a macrocyclic glycan with a characteristic three-dimensional torus shape [1]. Using CO-functionalized AFM probes, the sugar units of individual β-cyclodextrins can be clearly resolved, revealing the molecule's different adsorption geometries and conformations on the Au(111) surface. The position of individual hydroxy groups and the location of the stabilizing intramolecular H-bonds are deduced from atomically resolved images, enabling the unambiguous assignment of β-cyclodextrin's atomic structure.

Our results show the potential of combining electrospray deposition with non-contact AFM to resolve the atomic structure of single glycans, and could promote the application of this method to study various other biomolecules with atomic-scale detail.

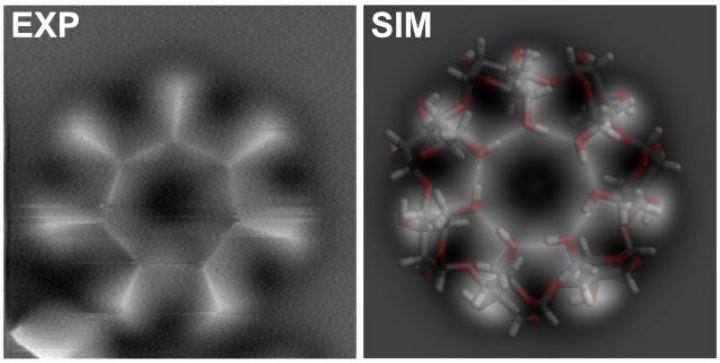

Figure – Experimental (left) and simulated (right) nc-AFM image of a single β-cyclodextrin molecule. DFT model is overlaid on the simulated image to aid visual assignment of the underlying structural elements.

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Nanoscale dielectric imaging of cells and bacteria by scanning dielectric microscopy assisted by deep convolutional neural networks

M. Cano [1,2], M. Checa [3], R. Millan-Solsona [3], G. Gomila [1,2]

[1] Department of Electronics and Biomedical Engineering, Universitat de Barcelona, Barcelona, Spain
[2] Nanoscale Bioelectrical Characterization, Institute for Bioengineering of Catalonia, Barcelona, Spain
[3] Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, USA.

mcano@ibecbarcelona.eu

The computational demand for processing electrical images in Scanning Dielectric Microscopy (SDM) is particularly high, sometimes requiring weeks or even months to complete due to the complexity of the models employed and the high volume of data to process. This creates a need for methods that can accelerate the data processing workflow, and artificial intelligence can be an adequate tool for this purpose. Techniques such as Multilayer Perceptrons have been previously used to model and replicate the processes involved in SDM data simulations. This work proposes the use of Convolutional Neural Networks (CNNs), known for their proficiency in image processing, in combination with a point-by-point Deep Neural Networks (DNN). This model allows for the consideration of point-specific electrical and topographical data, while also taking into account information from its surroundings resulting in a better contextualization of each point within the image.

This proposed neural network is trained using data derived from calculations of experimental data and has a high level of accuracy when replicating the calculation outcomes, even when trained with small datasets. By training this model with data curated for its intended application, it is possible to obtain pre-trained models that only require fine tuning to achieve accurate predictions. This reduces even further the amount of data that is needed and thus the total execution time. The application of this methodology in eukaryotic and bacterial cells is demonstrated, showing the potential of this approach for high throughput nanoscale dielectric imaging of biological samples and for its overall contribution to the development of multiparametric AFM methods.

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Patterning of graphene and MoS_2 devices by thermal scanning probe lithography

Y. K. Ryu [a,b], J. Martinez [c,b]

[a] Departamento de Física Aplicada e Ingeniería de Materiales, E.T.S.I Industriales, Universidad Politécnica de Madrid, C/José Gutiérrez Abascal 2, 28006 Madrid, Spain
[b] Instituto de Sistemas Optoelectrónicos y Microtecnología, Universidad Politécnica de Madrid, Av. Complutense 30, 28040 Madrid, Spain
[c] Departamento de Ciencia de Materiales-CIME, E.T.S.I Caminos, Canales y Puertos, Universidad Politécnica de Madrid, C/ Profesor Aranguren s/n, 28040 Madrid, Spain

* y.ryu@upm.es

Thermal scanning probe lithography (t-SPL) is a markerless, direct writing technique that allows to define patterns with high-resolution and free geometry in a wide range of materials, under ambient conditions. Its closed-loop lithography system makes possible the in-situ imaging and correction of writing parameters during the fabrication process. It enables grayscale lithography with nanometric resolution in the vertical direction. It has demonstrated an overlay accuracy of few nanometers and a field stitching accuracy of 25 nm.

In this talk, the patterning process of interdigitated electrodes on graphene and molybdenum disulfide (MoS_2) by applying t-SPL will be presented step by step to illustrate the features and capabilities of the technique to fabricate devices based on these materials at the nanoscale with high precision, low damaging, and reliability. The in-situ definition of electrical contacts directly on a chosen MoS_2 flake, without the need of prefabricated localization markers will be also shown to demonstrate the potential to fabricate devices based on 2D materials with a reduced number of steps.

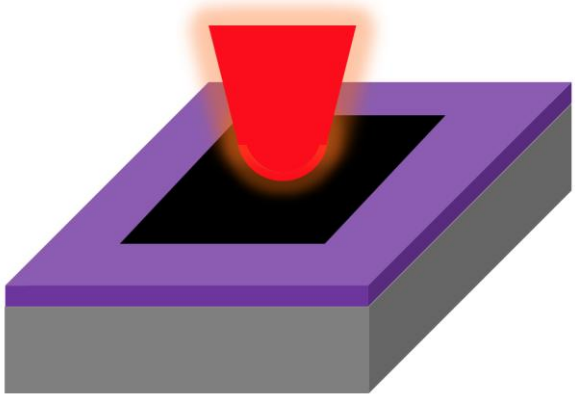

Figure – The minute tip in thermal scanning probe lithography acts as a hot pencil that draws all the devices one needs to fabricate on graphene and other 2D materials.

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2D Monolayer Nanotip Coating

Aitor Zambudio [a,b,c,*], Guillermo López-Polín [a], Pablo Ares [a,c], Jaime Colchero[b], Julio Gómez-Herrero [a,c], Cristina Gómez-Navarro [a,c]

[a] Dept. Física de la Materia Condensada, Univ. Autónoma de Madrid, 28049 Madrid, Spain.
[b] Centro de Investigación en Óptica y Nanofísica (CIOyN), Univ. de Murcia, 30100 Murcia, Spain.
[c] Instituto de Física de la Materia Condensada (IFIMAC), Univ. Autónoma de Madrid, 28049 Madrid, Spain.

* aitor.zambudio@uam.es

Functionalization of AFM tips has attracted attention in the last decades. The discovery of atomically thin 2D materials has broadened the field[1] as it has opened a new landscape in the ability to custom manipulate the electrical, tribological, wetting or quantum[2] properties of the probes apex beyond molecular functionalization, to name a few.

Here we describe a systematic and reproducible method for coating AFM nanoprobes with any desired 2D material. This procedure combines 2D material deposition on hole-patterned substrates, nanocutting, and tip-fishing. We report on the tuning of the different parameters involved to improve the reliability of the method, prove its versatility for different tip materials and 2D layers and test the maximum success rate in optimal conditions. To give an example, these covered tips will open new possibilities to probe 2D-2D materials nanotribology.

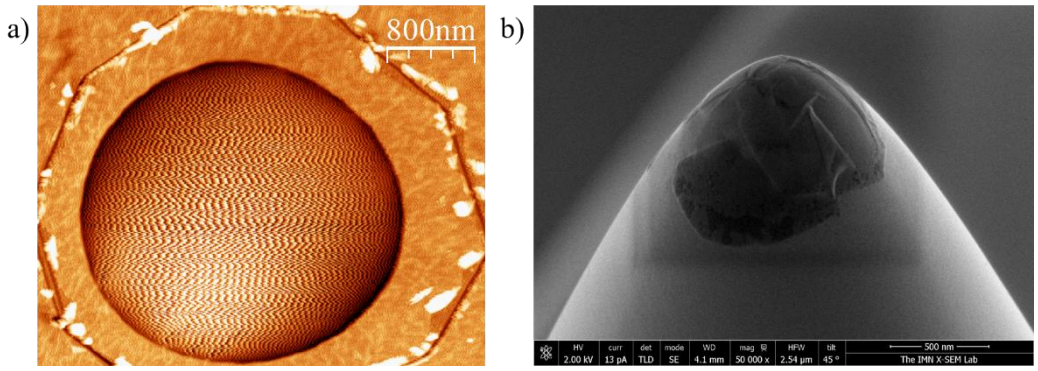

Figure 1 - a) AFM topography image of a cut MoS_2 flake that is suspended in a circular drum. b) Silicon tip apex coated with a monolayer MoS_2.

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Controlling spin ½ interactions in graphene: from quantum entanglement to altermagnetism

B. Viña-Bausá [a], R. Carrasco [a], M. A. García-Blázquez [a], S. Chourasia [a], E. Cortés-del-Río [a], A. T. Costa [b], D. Expósito [a], J. C. G. Henriques [b], P. Mallet [c], J.-Y. Veuillen [c], J. J. Palacios [a, d], J. Fernández-Rossier [b], I. Brihuega [a, d]

[a] Departamento de Física de la Materia Condensada, Universidad Autónoma de Madrid, E-28049 Madrid, Spain
[b] International Iberian Nanotechnology Laboratory, 4715-330, Braga, Portugal
[c] Université Grenoble Alpes, CNRS, Institut Néel, 38042, Grenoble, France
[d] Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, E-28049 Madrid, Spain

* beatriz.vina@uam.es

The ability to control spin coupling at the atomic scale is crucial both for fundamental studies and future applications in spintronics and quantum information. Here, we demonstrate that graphene, when functionalized with hydrogen (H) atoms, serves as a versatile platform for engineering and investigating long-range magnetic interactions. Through scanning tunneling microscopy (STM), we manipulate spin-1/2 moments induced by individual H atoms on graphene [1, 2] in order to build magnetically coupled structures, and quantify their coupling via spin excitations using inelastic electron tunneling spectroscopy (IETS) [3]. Our measurements reveal robust ferromagnetic and antiferromagnetic exchange interactions in H pairs, extending over nanometer-scale distances. Furthermore, we explore the emergence of tripartite quantum entanglement in H trimers and establish a direct link between inelastic spectral features and genuine multipartite entanglement. Additionally, guided by symmetry selection, we realize unconventional magnetic phases in our system [4], namely altermagnets [5] and Lieb ferrimagnets. Our experimental results are supported by mean-field Hubbard and density functional theory calculations (DFT). All these findings put forward hydrogenated graphene as a promising quantum material for simulating exotic spin systems and advancing quantum information technologies.

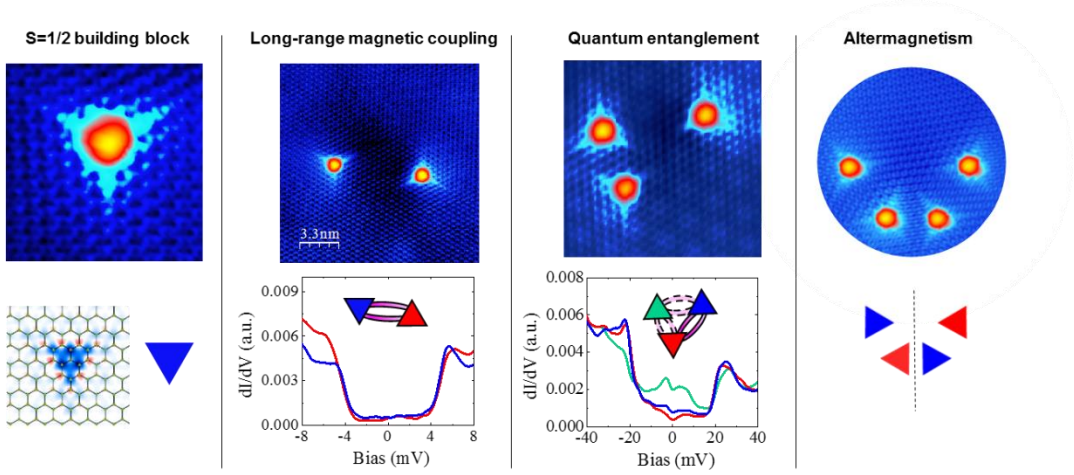

Figure – Using H atoms on graphene as S=1/2 building blocks, manipulated and probed at the atomic scale by STM and IETS, we can investigate long-range magnetic coupling, tripartite quantum entanglement and engineer novel, unconventional magnetic phases: altermagnets and Lieb ferrimagnets.

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Newly developed UHV-LT-Transport-STM/AFM system. From macro to nano in 10 minutes

D. Expósito [a], I. Brihuega [a,b]

[a] Dep de Física de la Materia Condensada, Universidad Autónoma de Madrid, Madrid, Spain
[b] Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, Madrid, Spain

* diego.exposito@uam.es

Since their first isolation, 2D materials have shown tantalizing properties at both the local and global scales. Scanning Probe Microscopy (SPM) techniques, and transport measurements, have produced, independently, exciting findings in these unique materials.
In our group, we have focused on studying the inherent graphene properties at the atomic scale by Scanning Tunneling Microscopy (STM). In addition to exploring graphene exotic properties [1], leveraging our expertise in UHV techniques, we are capable of systematically adding and tuning new properties. Specifically, we have demonstrated that we are able to induce superconductivity by proximity effect in graphene by growing Pb islands [3] and to induce local magnetic moments by selectively depositing single H atoms [4]. As a next critical step, we aim to externally tune these locally induced properties via electrostatic gating, enabling precise in situ adjustments of carrier density and direct correlations between atomic-scale modifications and global transport response. Two essential components are required to achieve such goal: an experimental tool providing access and control to graphene devices at the atomic scale, and an ultra-clean gateable graphene device. To this end, we have made two groundbreaking achievements.
First, we have developed a new microscope working in ultra-high vacuum (UHV) and low temperature (LT) capable of landing, within 5 µm accuracy, on specific regions of a few-micron-sized 2D flake in under five minutes. We can characterize samples both by means of STM and AFM, and continuously tuning the sample's electronic doping via an external gate.
Second, we have developed protocols to fabricate ultra-clean graphene devices, consisting in exfoliated monolayer graphene (MLG) flakes transferred on hexagonal boron nitride (hBN). STM images of these devices show atomically clean surfaces, fulfilling UHV standards.
In this context, here we show our ability to tune the doping of a graphene flake, and to deposit hydrogen atoms and led islands on the same sample. Additionally, we demonstrate our capability to precisely revisit previously AFM-mapped 10×10 µm² regions on samples provided by collaborating groups, enabling high resolution STM characterization of the exact same regions at 4 K in ultra-clean environments.

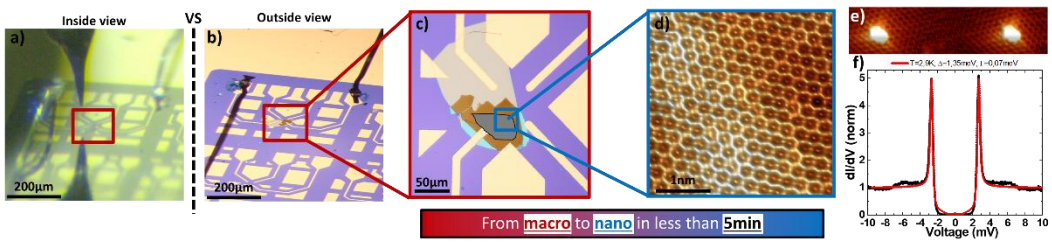

Figure 1. ***a)****,* ***b)*** *Long (Short) focal distance optical microscope photos of the MLG-hBN device inside (outside) the UHV chamber.* ***c)*** *Close-up of photo b).* ***d)*** *Atomic-resolution STM image of its surface.* ***e)*** *Single H atoms deposited on the device.* ***f)*** *Superconducting gap measured on evaporated Pb islands.*

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Atomically sharp 1D interfaces in 2D lateral heterostructures of VSe2-NbSe2 monolayers

Xin Huang[a], **Héctor González-Herrero**[a,b], Orlando J. Silveira[a], Shawulienu Kezilebieke[c], Peter Liljeroth[a], Jani Sainio[a],

[a] Department of Applied Physics, Aalto University, FI-00076 Aalto, Finland
[b] Departamento Física de la Materia Condensada,
Universidad Autónoma de Madrid, Madrid E-28049, Spain
[c] Department of Physics, Department of Chemistry and Nanoscience Center,
University of Jyväskylä, FI-40014 University of Jyväskylä, Finland.

*hector.gonzalez@uam.es

Van der Waals heterostructures have emerged as an ideal platform for creating engineered artificial electronic states. While vertical heterostructures have been extensively studied, realizing high-quality lateral heterostructures with atomically sharp interfaces remains a major experimental challenge.

In this work, we demonstrate a one-pot two-step lateral epitaxy technique to fabricate atomically sharp and well-defined lateral heterostructures of 1T-VSe_2—1H-$NbSe_2$ by molecular beam epitaxy (MBE) [1]. We demonstrate the formation of defect-free lateral heterostructures by low-temperature scanning tunneling microscopy (STM) and identify two different 1D interface structures corroborated by density-functional theory (DFT) calculations. Using scanning tunnelling spectroscopy (STS) we characterize their electronic structure. Our results point to the presence of 1D interfacial states as well as possible signatures of Kondo resonances in a side-coupled geometry.

This work demonstrates the full potential of lateral heterostructures for achieving complex lateral heterostructures with atomically well-defined 1D interfaces where it is possible to realize correlated many-body states via lateral coupling through the right choice of materials.

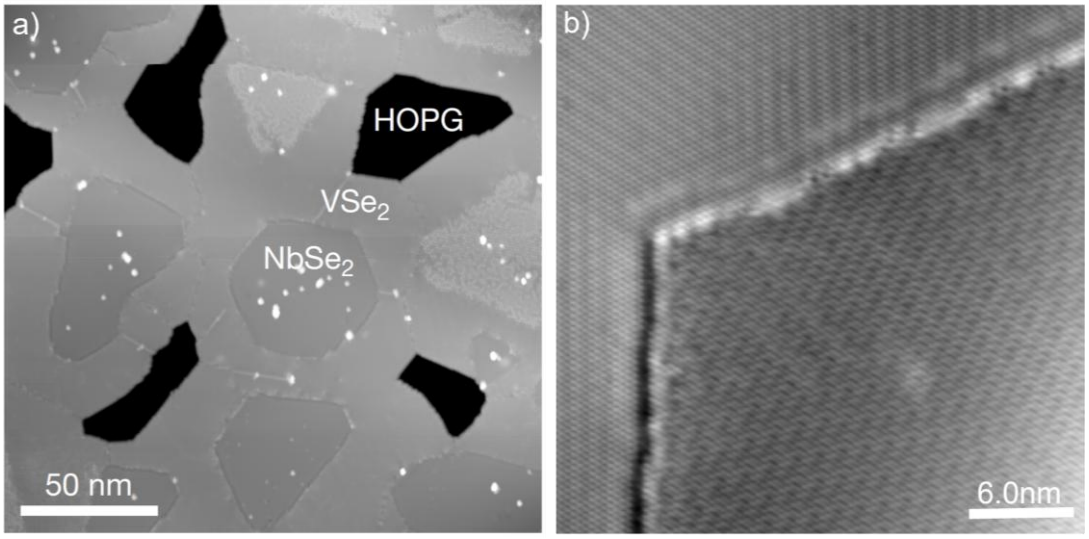

Figure - VSe2-NbSe2 lateral heterostructures. a) STM image of our typical sample grew with our MBE method. b) Zoom in of one of the heterostructures.

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The synergy of scanning probe microscopy and 2D materials to advance nanocatalysis

A. J. Martínez-Galera [a,b,c]

[a] Departamento de Física de Materiales, Universidad Autónoma de Madrid, E-28049 Madrid, Spain
[b] Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, E-28049 Madrid, Spain
[c] Instituto Nicolás Cabrera, Universidad Autónoma de Madrid, E-28049 Madrid, Spain

* antonio.galera@uam.es

Catalysis is a cornerstone of various research areas and of modern industry, underpinning over 90% of global production across various sectors, including chemicals and energy. As the demand for more efficient and sustainable catalytic processes intensifies, a deeper understanding of the atomic-scale phenomena occurring on the surface of the nanocatalysts becomes essential.

This presentation intends to highlight the potential of the scanning probe microscopies, which are able to investigate matter in real space with atomic resolution, to address a key challenge in heterogeneous catalysis: achieving access to the atomic-scale processes taking place in the nanocatalysts. Moreover, it is also aimed to underline the prospects of 2D materials as inert supports for the development of nanocatalysts with tunable size and composition [1, 2]. Specifically, the focus will be on three main aspects. First, the presentation will cover the generation of suitable supports for nanoparticle growth from 2D materials by their functionalization through ion bombardment. Next, it will delve into the effects of nanoparticle growth on the structural properties of these 2D material supports [3]. Afterwards, it will tackle the study of the internal atomic restructuring that occurs in nanocatalysts during their involvement in the reaction [4, 5]. Finally, the presentation will provide a brief overview of our ongoing project aimed at achieving atomic-scale visualization of the processes occurring along the reaction pathway.

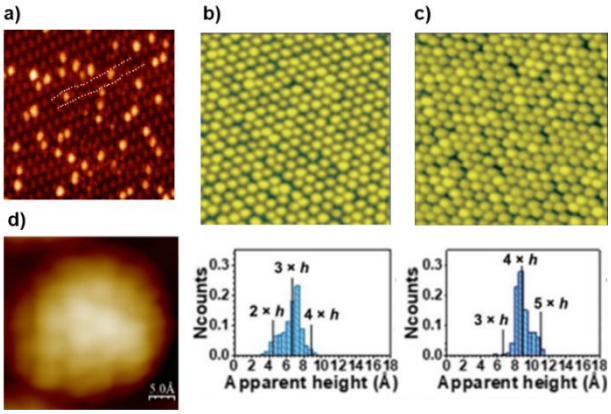

Figure - **a)** STM image revealing moiré pattern distortion after the growth of Si nanoparticles on graphene/Ru(0001). **b) c)** STM images showing the spatial distribution of Ir nanoparticles grown on h-BN/Rh(111) before (b) and after (c) O_2 exposure at elevated temperatures (top panels), and apparent height histograms obtained for each case (bottom panels). **d)** STM image displaying the surface of a nanocatalyst with atomic resolution. Size of the STM topographs: 50 × 50 nm^2 for a), b), c), and 3 × 3 nm^2 for d).

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Frictional Contrast of Atomic Defects: A Combined LFM and MD Approach

Oscar Gutiérrez-Varela[a,b*], Aitor Zambudio[c], Pablo Ares[c], Julio Gómez-Herrero[c], Cristina Gómez-Navarro[c], and J.G. Vilhena[a*]

[a]Instituto de Ciencia de Materiales de Madrid, Consejo Superior de Investigaciones Científicas, Madrid, Spain
[b]Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, Madrid, Spain
[c]Departamento de Física de la Materia Condensada, Universidad Autónoma de Madrid, Madrid, Spain

*oscarj.gutierrez@uam.es, guilherme.vilhena@csic.es

MoS_2, a prominent transition metal dichalcogenide (TMD), is extensively studied for its promising applications in electronics, optoelectronics, and catalysis [1]. However, defects in MoS_2 can significantly affect its performance, making precise defect characterization essential [2]. Lateral Force Microscopy (LFM), a widely used mechanical technique, enables the detection of frictional changes at the atomic scale, offering a practical approach for routine defect detection with minimal technical complexity [2,3]. In this study, we combine LFM with Molecular Dynamics (MD) simulations to assess its ability to detect atomic vacancies in MoS_2. Our results show that LFM can capture distinct frictional signatures associated with both surface and sub-surface vacancies. Importantly, LFM demonstrates the sensitivity necessary to detect defects at the atomic scale, in line with the predictions from MD simulations, highlighting its potential for defect characterization in TMDs. Furthermore, we show that LFM can distinguish between surface and sub-surface vacancies based on their contrast in the frictional maps. However, chemically distinguishing different types of vacancies within each group remains a challenge. Our results provide a robust validation of LFM's potential for routine atomic defect characterization in TMDs, paving the way for more comprehensive defect analysis in 2D materials.

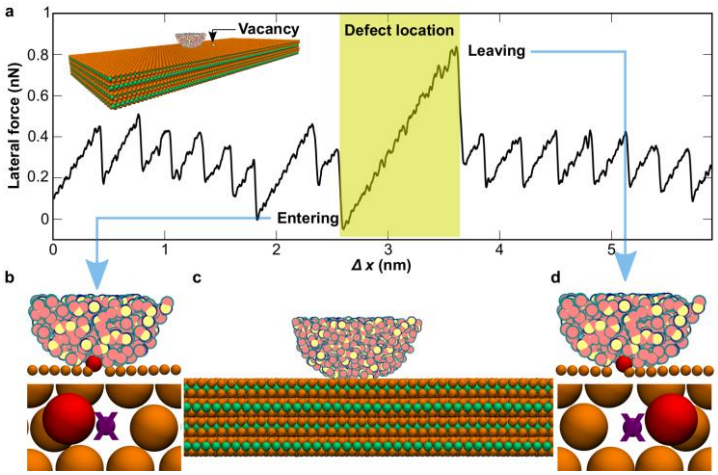

Figure – Molecular system under investigation and lateral force trace showing the presence of a surface atomic vacancy.

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Atomic-Scale Investigation of the CeO_2(100) Surface using Atomic Force Microscopy and Force Spectroscopy

Kyungmin Kim[a*], Oscar Custance [b], Masayuki Abe [a], Shigeki Kawai [b]

[a] Osaka University, 1-3 Machikaneyama, 560-8531 Toyonaka, Japan
[b] National Institute for Material Science (NIMS), 1-2-1 Sengen, 305-0047 Tsukuba, Japan

* u764704g@ecs.osaka-u.ac.jp

Cerium dioxide (ceria, CeO_2) plays a crucial role in catalysis, primarily due to its remarkable oxygen storage capacity [1]. The surface of ceria-based catalysts comprises various CeO_2 nano-facets, making the study of different crystal orientations highly relevant. Among the low-index surfaces of ceria, the CeO_2(100) orientation is regarded as the most reactive [2]. However, the inherent polarity of the CeO_2(100) surface, combined with strong electrostatic repulsion between exposed atoms, often leads to structural reconstructions, adding complexity to the interpretation of experimental observations [3].

In this work, well-defined CeO_2(100) thin films were grown on a Cu(111) substrate. We performed Scanning Tunneling Microscopy (STM) and high-resolution Non-Contact Atomic Force Microscopy (NC-AFM) with force spectroscopy under ultra-high vacuum, and at 4.8 K. Figure 1(a) shows a high resolution STM image of a multilayer CeO_2(100) island grown on a Cu oxide substrate. The topmost CeO_2(100) island exhibit a (2 x 2) surface reconstruction, whereas the atomic layer underneath exhibits a c(2 x 2) reconstruction. Figure 1(b) shows a high resolution AFM image of (2 x 2) reconstruction with atomic defect. We thoroughly explore the atomic structure of the CeO_2(100) surface by combining site-specific force spectroscopy with well-established DFT theoretical models [3-5].

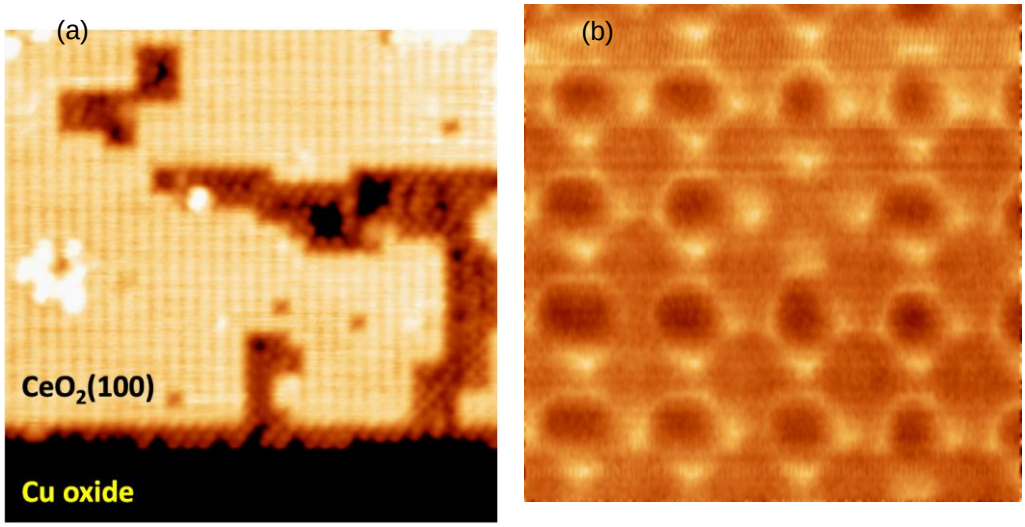

Figure 1. (a) High resolution STM image of a multilayer CeO_2(100) island grown on a Cu(111) substrate. (b) High resolution AFM image of CeO_2(100)-(2x2) surface reconstruction with atomic defect.

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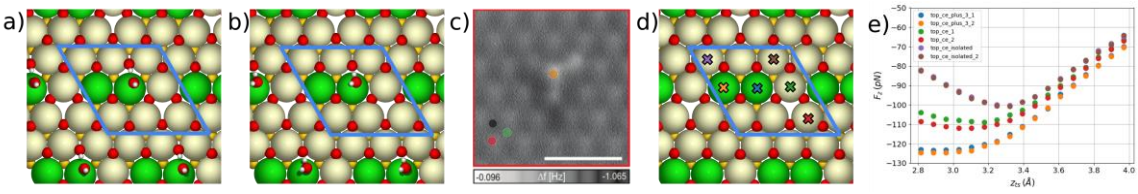
Identifying Ce^{3+} sites at the reduced CeO_2 (111) surface: the role of water molecules and AFM imaging

M. González Lastre*[, a], O. Custance*[, b], K. Kim [c], E. Fernandez-Villanueva [d], P. Pou [a,e], H. Sepehri-Amin [b], D. Katsube [f], M. Abe [c], S. Kawai [b], M. V. Ganduglia-Pirovano [d], R. Pérez [a,e]

[a] Dept de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, E-28049 Spain
[b] National Institute of Materials Science (NIMS), Tsukuba, Japan
[c] Graduate School of Engineering Science, Osaka University Toyonaka, Osaka 560-0043, Japan
[d] Instituto de Catálisis y Petroleoquímica (ICP-CSIC), E-28049 Spain
[e] Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, E-28049 Spain
[f] Surface and Interface Science Laboratory, RIKEN, Hirosawa 2-1, 351-0198 Wako, Saitama, Japan
* manuele.gonzalez@uam.es

Significant experimental and theoretical efforts have been made to determine the most energetically favourable configuration for O vacancies and the associated reduced Ce^{3+} sites at ceria (CeO_2) surfaces. While carbon monoxide, CO, coupled with IR spectroscopy presents a promising method for surface probing [1], the precise assignment of the different CO vibrational bands remains complex [2]. Building upon previous work on the (101) anatase surface [3], we propose an alternative approach for identifying Ce^{3+} sites. Our method combines experiments using water as a marker with Non-Contact Atomic Force Microscopy (NC-AFM) and sophisticated simulations of the NC-AFM images. NC-AFM, using metal tips functionalized with closed-shell molecules like CO or with an O-terminated Cu tip obtained by soft nano indentation, yields images with truly unprecedented resolution. Previous AFM measurements (based on silicon cantilevers) of adsorbed water revealed a triangular symmetry as predicted by us [4]. However, recent NC-AFM experiments at NIMS, employing O-terminated tips and small oscillation amplitudes using stiff piezoelectric cantilevers, reveal a boomerang-like shape of water molecules spanning two of the three equivalent surface O sites. Additionally, these images exhibit a complex contrast on the surrounding areas. Detailed spectroscopy measurements provide clearly distinguishable force versus distance curves on different Ce and O sites both in the pristine surface and around the water molecule. DFT calculations motivated by these experiments, suggest a preferential binding of water, both in molecular and dissociated states, to Ce^{3+} sites over Ce^{4+} sites on the surface. Our hypothesis [5] suggests that water can serve as a marker for the location of Ce^{3+} and that nanomanipulation using a probe is feasible. This methodology holds promise for significantly advancing the characterization of catalyst surfaces based on ceria and other relevant oxide surfaces.



Schematic representation of dissociated (a) and molecular (b) water adsorption configurations, with the unit cell outlined in blue. (c) Experimental constant-height AFM image of a CeO_2(111) surface with adsorbed water. The three atomic sites of CeO_2 are identified: oxygen (red), cerium (white), and coordination vacancy (green), with water (orange) serving as a site marker. (d) Reduced CeO_{2-x}(111) surface sites with corresponding DFT force vs tip-surface distance curves (e). Ce^{3+} sites appear more attractive than Ce^{4+} atoms.

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Unraveling the anomalous dielectric properties of interfacial and nanoconfined water

Laura Fumagalli[a,b]*

[a] Department of Physics & Astronomy, University of Manchester, Manchester M13 9PL, UK
[b] National Graphene Institute, University of Manchester, Manchester M13 9PL, UK

*laura.fumagalli@manchester.ac.uk

In this contribution, I will talk about our work in which we experimentally investigate the dielectric polarization properties of near-surface and confined water. These properties have long been subject of research because they are critical to a variety of phenomena, including surface forces, ion/molecular solvation and transport, and chemical reactions. However, they have remained essentially unknown for great difficulties in measuring them. After briefly introducing our experimental setups that are based on advanced scanning probe methods [1-3], I will discuss our recent results in which we directly measured the dielectric properties of few water layers confined inside nanochannels made of van der Waals crystals [4,5]. Our experiments revealed the presence of an interfacial water layer with dielectric properties that greatly differ from those of bulk water. Our results open up new possibilities for understanding many natural processes, providing important feedback for theories describing water-mediated interactions.

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Calibration of Scanning Joule Expansion Microscopy for nanoscale heat transport studies

Jae Hwan Jeong [a,b,c], Diego A. Aldave [a,b,c], Julio Gómez-Herrero [a,b,c], Pablo Ares [a,b,c]

[a] Departamento de Física de la Materia Condensada, Universidad Autónoma de Madrid, Madrid, 28049, Spain
[b] Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, Madrid, 28049, Spain
[c] Instituto Nicolás Cabrera (INC), Universidad Autónoma de Madrid, Madrid 28049, Spain

* jeong.jaehwan@uam.es

Measuring nanoscale heat transport is an important aspect of current technological developments. Among atomic force microscopy (AFM) techniques, scanning thermal microscopy (SThM) is predominantly used for thermal property measurements. However, SThM has several limitations, including the need for expensive specially fabricated probes, customized instruments which has electrical circuits for the SThM probe, and lateral resolution lower than standard AFM measurements.[1]

Several alternative techniques have been explored to address the limitations of SThM. Among AFM-based thermal measurement methods, scanning joule expansion microscopy (SJEM)[2] stands out as a promising candidate for studying thermal properties at the nanoscale. SJEM measures the thermal properties of surfaces through thermal expansion. It offers several advantages, such as high lateral resolution due to the use of standard probes, ease of use, fast measurement, and versatile probe and instrument choices. These attributes make SJEM an attractive tool for studying heat transport, especially in two-dimensional (2D) materials.[3]

Despite its benefits, SJEM is a qualitative technique that provides relative information about heat transfer speed, making it challenging to obtain quantitative temperature data.

To address the hurdles limiting the wider adoption of SJEM, we aim to develop a calibration process to transform SJEM into a quantitative tool for studying heat transport processes. Various techniques, including Raman thermometry using silicon nanoparticles (Si NPs) and finite element method (FEM) simulations, are employed to achieve this goal.

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Nanoscale wetting characterization using non-contact Scanning Probe Microscopy in humid conditions

P. Sudersan [a], J. Colchero [a]

[a] Department of Physics, University of Murcia, Spain

* p.sudersan@um.es

Wetting of liquid drops on a solid surface is fundamental to many biological and industrial processes. Typically, wetting is characterized by its macroscopic contact angle. However, nano-scale chemical and topographic heterogeneities of the surface profoundly affect the macro-scale contact angle measurements. Here, we demonstrate that non-contact Dynamic Atomic Force Microscopy (DAFM) can be a valuable tool for characterizing the wetting of water on surfaces at the nano-scale. It is known that under humid conditions, an AFM tip close to a surface causes the spontaneous condensation of a water meniscus between the tip and the surface [1,2]. Interestingly, the resulting capillary interactions have both conservative and dissipative components that depend on the nano-scale contact angle of water with the surface. Typically, capillary force causes the tip to snap to contact. However, when the cantilever is oscillated (as in DAFM), not only does the tip avoid snap-in, but rather, it manages to avoid any hard contact with the surface altogether. The temporary dissipative interaction experienced by the tip due to condensation, which occurs only when the instantaneous tip-sample distance during an oscillation cycle is below a particular length, causes the cantilever's oscillation amplitude to pulsate and avoid contact. This is shown by experimental amplitude-distance curves made on hydrophilic (mica) and hydrophobic (HOPG) samples, as well as numerically simulating the cantilever's non-linear harmonic response to such interactions (Figure 1). Operating the DAFM at constant phase using a phase locked loop (PLL) allows separating the conservative and dissipative parts of the total interaction, where, the "frequency shift" channel contains information related to the local van der Waals and capillary interaction, while, the "amplitude" channel is related to the purely dissipative component of the capillary interaction. In the manner, the local nano-scale wetting property of the surface can be mapped out, while avoiding tip-sample contact. This approach is tested by performing measurements on interdigitated electrode samples, where the gold electrodes were selectively functionalized with thiols. Such a model sample provides us with micro-scale hydrophobic (thiol-coated gold) and hydrophilic (glass) regions, whose wetting properties can be characterized in a single AFM scan image.

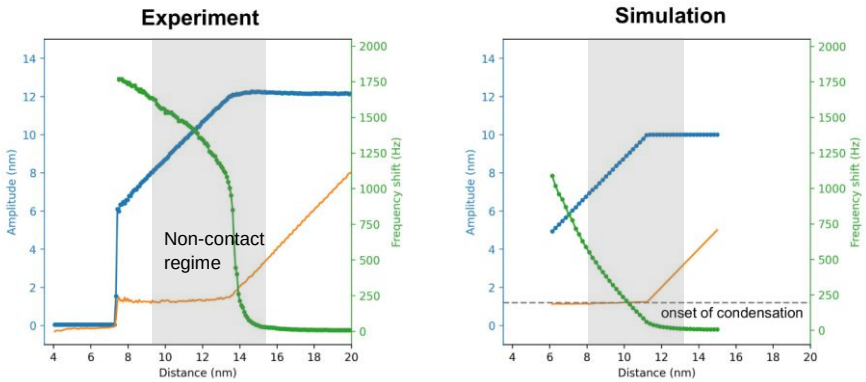

Figure 1 – Experimental vs simulated interaction-distance curves on mica. Orange curves show that the tip-sample distance at the lower turning point of oscillation is not zero in the "non-contact" regime

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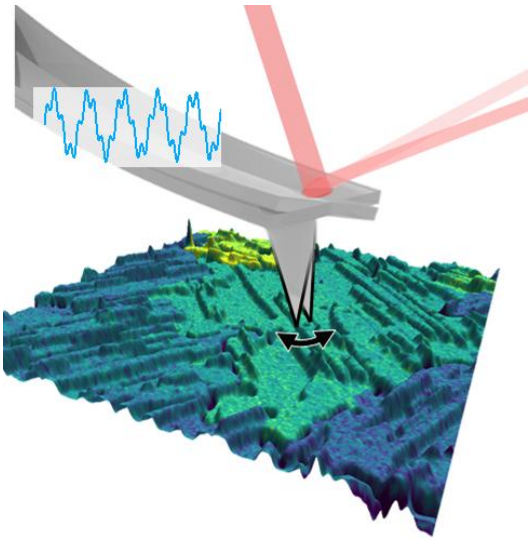
Bimodal atomic force microscopy with a torsional eigenmode for highly accurate imaging of grain orientation in organic thin films

R. Arilla, E. Barrena, C. Ocal, **D. Martin-Jimenez**

Institut de Ciència de Materials de Barcelona (ICMAB), CSIC, Campus Bellaterra 08193, Barcelona, Spain

* daniel.martin@csic.es

In organic electronics, the nature and spatial distribution of grains in polycrystalline thin films of small organic semiconductor molecules greatly impact the electronic properties of devices. Therefore, tools that accurately characterize organic films at the mesoscopic level are essential. To this end, we demonstrate here the power of a bimodal Atomic Force Microscopy (AFM) with a torsional eigenmode for highly accurate imaging grain orientations in organic thin films. The energy dissipated between tip and sample during scanning depends on the in-plane crystalline orientation of each grain. This fact alters the cantilever torsional observables, allowing grain orientation recognition. Remarkably, bimodal AFM with the torsional eigenmode has important advantages, such as high sensitivity in the applied forces, true molecular resolution, and multiple parameters for regulating the image contrast, making it competitive with other well-established AFM methods for grain detection in organic thin films, namely Friction Force Microscopy and Transverse Shear Microscopy.



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Jumping Mode++ (Touch & Go)

I. Horcas [a], A. Díez-Martínez [a], P. Ares [a], P. J. de Pablo [a], J. Gómez-Herrero [a]

[a] Departamento de Física de la Materia Condensada & Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, Madrid 28049, Spain

* ignacio.horcas@uam.es

Atomic Force Microscopy Jumping Mode (AFM-JM)[1,2] using WSxM[3] was the first off-resonance controlled intermittent contact method designed to avoid lateral forces while controlling the tip-sample interaction, allowing measurement of soft samples weakly fixed to the substrate. JM+[2] is an optimized version of JM for liquid measurements, compensating hydrodynamic drag forces and therefore improving the tip-sample detection and minimizing applied forces. While the results obtained using JM and JM+ during these years demonstrate the adequation of them for scanning soft biological samples[4], the acquisition time has always been an important drawback.

In this work we introduce Jumping Mode++ (JM++ Touch & Go), which improves off-resonance modes by reducing the acquisition time and avoiding some artifacts such as the commonly known parachuting effect. This is an artificial shadow in the images (see Figure 1 left) that appears when the tip descends from a high feature in the image. In these regions, classic JM methods start and finish the acquisition of an image point and then activate a feedback control loop that looks for the contact point by measuring the normal force, modifying the Z scanner extension to reach a desired normal force setpoint. The time period this loop remains active is user-configurable and affects the total acquisition time and the quality of the image. JM++ Touch & Go reduces, or even removes, the need of the feedback loop when descending high features by extending the Z displacement until the sample surface is detected, greatly reducing acquisition times and parachuting artifacts (see Figure 1 right). This requires a modification of the classical sinusoidal waveform used to avoid the ringing effect caused by high accelerations. Instead of that, we use a rounded triangular wave, mixing a constant speed for the sample detection and an initial retract with a soft change of direction to minimize the acceleration and the ringing effect.

JM++ Touch & Go will allow following dynamic processes with excellent control of the applied forces, both normal and lateral. Besides, it will provide mechanical properties maps such as adhesion or stiffness.

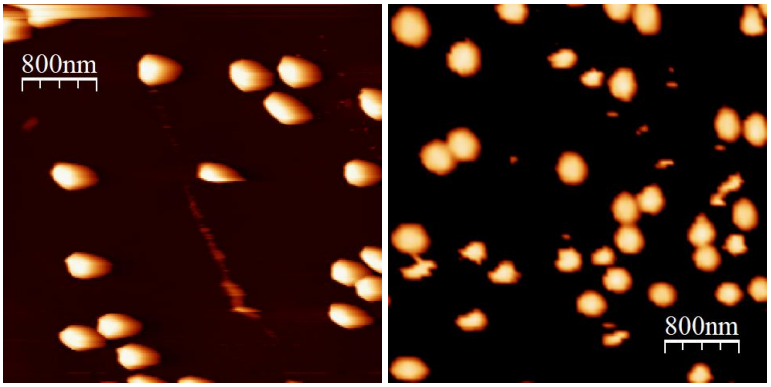

Figure 1 – Images of viral particles comparing the parachuting effect in JM+ (left) and JM++ (right)

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Photochemical reactions on a semiconducting surface

Ana Sánchez-Grande,[a,b] Federico Frezza,[a] Sofia Canola,[a] Anna Lamancová,[c] Karl-Heinz Ernst,[a] Marco Di Giovannantonio,[d] Dana Nachtigallová[c] and Pavel Jelínek[a]

[a] Institute of Physics, The Czech Academy of Sciences, Cukrovarnická 10, 162 00, Prague 6, Czech Republic.
[b] Departamento de Química Orgánica, Facultad de Química, Universidad Complutense, E-28040 Madrid, Spain
[c] Institute of Organic Chemistry and Biochemistry Czech Academy of Science Flemingovo náměstí 542/2, 160 00 Prague, Czech Republic.
[d] Istituto di Struttura della Materia CNR (ISM-CNR) via Fosso del Cavaliere 100, 00133, Rome, Italy.

ana.sanchez@fzu.cz , anasan02@ucm.es

The on-surface synthesis (OSS) approach has been demonstrated to be a very powerful strategy to synthesize diverse carbon-based nanomaterials, presenting remarkable magnetic and electronic properties, and with the goal of integrating them into electronic devices. So far, the OSS field has been developed on metallic surfaces, exploiting their catalytic properties to open new reaction pathways toward synthesizing new carbon-based nanomaterials precluded by solution chemistry. However, the reliance on metallic substrates in OSS restricts these nanomaterials' applications, necessitating strategies for transferring these materials into technologically relevant substrates. Direct synthesis on non-metallic surfaces presents some limitations, mainly related to the low adsorption energies of the molecular precursors and the lack of catalytic activity from the substrate. Addressing these limitations, we explore the field of on-surface photochemistry as an alternative to thermally induced reactions, enabling controlled chemical processes at lower temperatures.

Here, we present different examples of light-driven on-surface reactions on a SnSe surface. We explore the photoreactivity of different molecules, focusing on the mechanisms triggering the reaction upon irradiation. In the case of the anhydride-based molecules,[1] we show that photodissociation is initiated by the presence of a n→π* first excited state with strong dissociative character. Additionally, we demonstrate how changes in the π-conjugation of the molecular core or in the geometry imposed by the 2D surface have an impact in the order of the excited states and hence in the photoreactivity. Secondly, we investigate the family of cyclopropenone-based molecules, whose photoactivity relies on ultrafast reactions.[2] The experimental scanning probe microscopy results were corroborated by quantum chemical calculations.

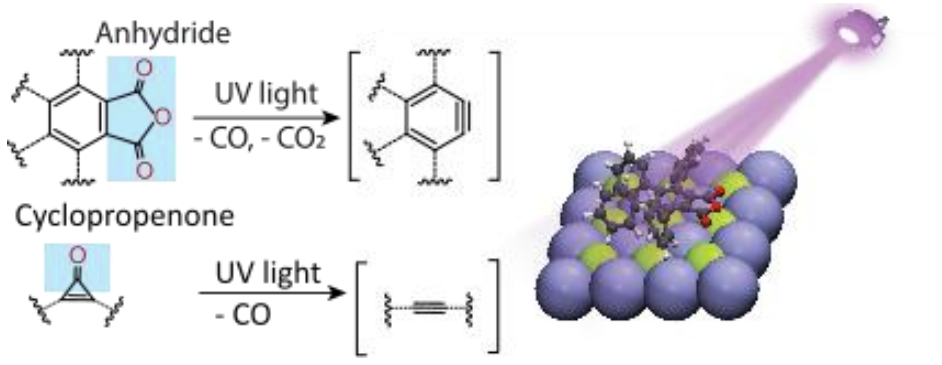

Figure. Chemical sketch of photochemical reactions on a SnSe surface.

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On-surface light vs thermal synthesis of a porous network

V. Villalobos-Vilda [a], **E. Tosi** [a], B. Carli [b], L. Marzo [b], S. Cabrera [b], M. F. López [a], J. Alemán [b], J. A. Martín-Gago [a], C. Sánchez-Sánchez [a]

[a] Instituto de Ciencia de Materiales de Madrid (ICMM-CSIC), C/Sor Juana Inés de la Cruz 3, 28049, Madrid, Spain

[b] Departamento de Química Orgánica (Módulo 1), Facultad de Ciencias, Universidad Autónoma de Madrid, C/Francisco Tomás y Valiente 7, 28049, Madrid, Spain

* ezequiel.tosi@csic.es

On-surface synthesis enables the formation of extended polymeric networks with tailored properties, offering new avenues for functional materials in catalysis and optoelectronics. While thermally-induced polymerization has been widely explored, achieving precise control over reaction pathways remains challenging, particularly on technologically-relevant substrates. Previous studies have demonstrated that light-driven polymerization can provide an alternative route to thermally inaccessible reactions [1], which can be of particular importance in non-metallic surfaces [2]. In this study, we investigate the on-surface photopolymerization of a molecular precursor – composed of three ester groups and three α, β unsaturated carbonyl groups – on Au(111) and the α- and β-phases of SnSe under ultra-high vacuum conditions, paying special attention to the comparison with thermal activation. Our results show that while thermal annealing on Au(111) leads to the formation of a porous network, on SnSe the molecules desorb from the surface before polymerization. Remarkably, triggering the reaction by illumination enables the formation of the porous network on β-SnSe, overcoming the thermal constraints observed on this surface. These findings provide new insights into the design of photochemically synthesized 2D polymers, expanding their applicability beyond metal substrates and opening new possibilities for the fabrication of functional organic materials.

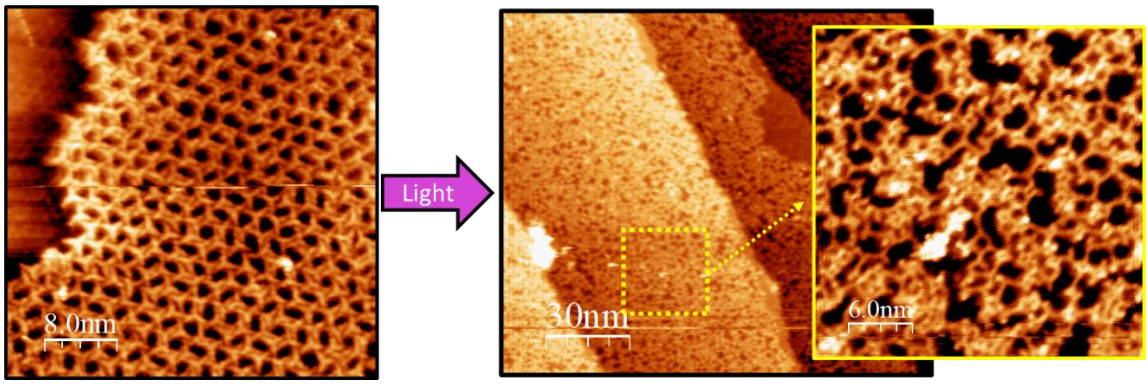

*Figure – STM images of the porous network obtained by the illumination of the self-assembly on **β**-SnSe*

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On-surface synthesis and characterization of [19]-starphene

S. Salaverría [a], J. Besteiro-Sáez [b], L. M. Mateo [b], T. Wang [c], P. Angulo-Portugal [d], J. P. Calupitan [e], A. García-Fuente [f], J. Rodríguez-Fernández [f], J. Ferrer [f], E. Guitián [b], D. Pérez [b], M. Corso [c,d], D. Peña [b], and D. G. de Oteyza [a,c]

[a] Nanomaterials and Nanotechnology Research Center (CINN), CSIC-UNIOVI-PA, 33940 El Entrego, (Spain)
[b] Centro de Investigación en Química Biolóxica e Materiais Moleculares (CiQUS) and Departamento de Química Orgánica, Universidade de Santiago de Compostela, 15782 Santiago de Compostela, (Spain)
[c] Donostia International Physics Center, 20018 San Sebastián, (Spain)
[d] Centro de Física de Materiales (CFM-MPC), CSIC-UPV/EHU, 20018 San Sebastián, (Spain)
[e] Institut Parisien de Chimie Moléculaire (IPCM) Sorbonne Université, CNRS F-75005 Paris, (France)
[f] Physics Department,University of Oviedo, 33007 Oviedo (Spain)

* s.salaverria@cinn.es

Starphenes are a family of star-shaped polyarylenes formed by the symmetric trimerization of acene molecules. Just like acenes, starphenes possess small HOMO-LUMO gaps and a limited number of Clar sextets regardless of their size (one per acene arm), endowing them a higher reactivity as their size increases. Their low solubility and high instability under ambient conditions presents significant synthetic challenges precluding their production. Recently, on-surface synthesis under ultra-high vacuum has emerged as an efficient approach to overcome these limitations [1], enabling the formation of novel molecular nanostructures.

In this presentation we will discuss recent advances in the synthesis and characterization of Starphene molecules on surfaces. Specifically, we will present the synthesis of [19]-starphene [2], the largest starphene fabricated to date, achieved through two distinct approaches. Atomic-scale characterization of the electronic and geometric structure of [19]-starphene is conducted via bond-resolved STM and conductance maps of the molecular orbitals. The experimental observations are fully supported by DFT calculations, enabling the assignment of the molecular orbitals and confirming a close-shell character. Our results unambiguously demonstrate a HOMO-LUMO gap of [19]-starphene of 0.9 eV [2], continuing the inverse length-dependence of the starphene arm and the band gap for close-shell configuration. According to theoretical calculations, the appearance of the open-shell character in starphenes once they increase in size results in a saturation of their bandgap to the same levels as in the long acenes, slowing down its bandgap decay. Importantly, the synthetic method to obtain [19]-starphene can be directly extrapolated to larger sizes, setting the base to characterize and confirm their pronounced multiradical properties predicted by calculations.

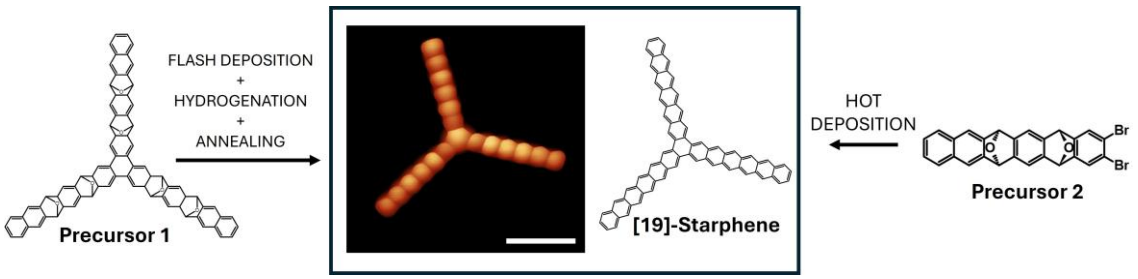

Figure- Schem of the two different starphene synthesis routes and a central BR-STM image (CO tip) of [19]- starphene.

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Globally aromatic odd-electron π-magnetic macrocycle

Federico Villalobos[a,g], Jan Berger[b,c], Adam Matěj[b,d], Reed Nieman[e], Ana Sánchez-Grande[b], Diego Soler[b], Hans Lischka[e], M. Matoušek[f], J. Brabec[f], L. Veis[f], Alba Millan[a], Carlos Sánchez-Sánchez[g], Araceli G. Campaña[a], Juan M. Cuerva[a] and Pavel Jelínek[b,c].

[a] Departamento Química Orgánica, Universidad de Granada (UGR), Unidad de Excelencia de Química UEQ, C. U. Fuentenueva, 18071 Granada, Spain.
[b] Institute of Physics of the Czech Academy of Sciences, Prague, Czechia.
[c] CATRIN-RCPTM, Palacký University Olomouc, Olomouc, Czechia.
[d] Department of Physical Chemistry, Faculty of Science, Palacký University Olomouc, Olomouc, Czechia.
[e] Department of Chemistry and Biochemistry, Texas Tech University, Lubbock, TX 79409-1061, USA.
[f] J. Heyrovský Institute of Physical Chemistry, Czech Academy of Sciences, Prague, Czechia.
[g] ESISNA Group, Instituto de Ciencia de Materiales de Madrid (ICMM-CSIC), Sor Juana Inés de la Cruz 3, 28049 Madrid, Spain.

* federicovr@ugr.es

Single organic molecule-based molecular π-magnets[1] have attracted significant interest due to their promising applications in optoelectronics and spintronics. Additionally, macrocyclic π-magnet molecules offer a fascinating platform for studying both magnetic and aromatic properties. However, the concept of global aromaticity in conjugated macrocyclic polyradicaloids remains largely unexplored, with existing studies mostly focused on molecules with an even number of electrons[2].

In this work[3], we report the on-surface synthesis of a cyclopenta-ring-fused oligo(m-phenylene) macrocycle, **9MC**, which contains an odd number of electrons. This polyradicaloid undergoes a surface-induced distortion, adopting a D_{3h} symmetry with a fully delocalized doublet ground state. Remarkably, **9MC** exhibits two aromatic annulene-within-an-annulene (AWA) ring currents within its inner and outer rings.

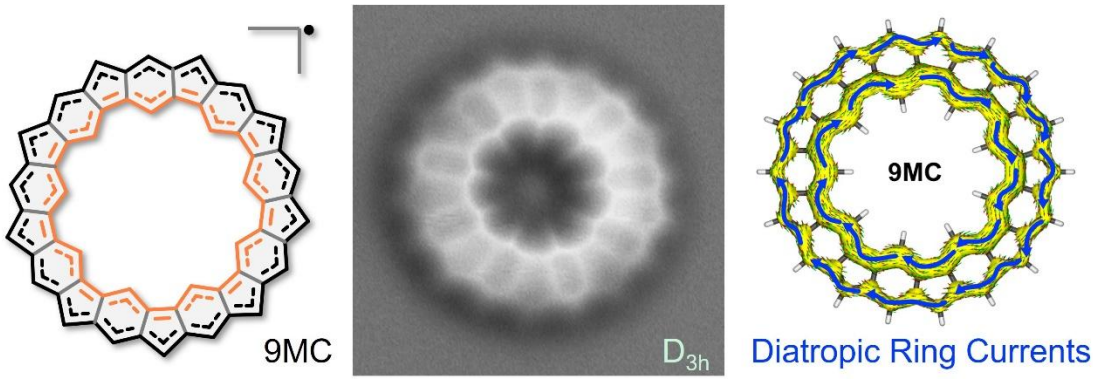

*Figure 1. **9MC** Macrocycle. From left to right, chemical sketch of the structure, nc-AFM image of the on-surface synthesized macrocycle, and ACID plot with both rings being diatropic.*

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Inducing radical states by nitrogen deprotonation in pyrrole bearing polycyclic hydrocarbons

E. Peláez-Sifonte [a], F. Villalobos Romero [b,c], Jesús I. Mendieta-Moreno [c], O. Stetsovych [d], J. Lobo-Checa [a], J.M. Cuerva [b], A.G. Campaña [b], P. Jelinek [d], J.I. Martínez [c], C. Sánchez Sánchez [c], D. Serrate [a,e]

[a] Instituto de Nanociencia y Materiales de Aragón, CSIC-Universidad de Zaragoza, Zaragoza, Spain
[b] Departamento de Química Orgánica, Universidad de Granada, Spain
[c] Instituto de Ciencia de Materiales de Madrid, CSIC, Spain
[d] Institute of Physics, Czech Academy of Sciences, Prague, Czech Republic
[e] Laboratorio de Microscopias Avanzadas, Universidad de Zaragoza, Spain

* epelaez@unizar.es

On-surface synthesis enables the synthesis of planar organic molecules on solid surfaces under ultra-high vacuum conditions. One of the most sought-after goals is to create artificial arrangements of the conjugated pi-electron cloud with one or several radical sites. To this end, dehydrogenation of carbon sites in non-benzenoid derivatives has proved an efficient pathway to stabilize poly-radical states on surfaces [1]. Here we show that controlled cleaving by an STM tip of hydrogen-nitrogen bonds in pyrrole bearing polycyclic hydrocarbons can also induce open-shell ground states with 1 to 4 coupled radical states, thus providing an ideal platform to study the correlation between structure and quantum spin phenomena. We report the sequential dehydrogenation of nitrogen sites in propeller shaped molecules (PSM) on selected coinage metal surfaces (Ag(001), Cu(001) and (Cu111)). We experimentally find that hydrogens can be individually cleaved via voltage pulses within the 1.2 V<V_{th}<2 V range in the three substrates. Interestingly, such cleaving proceeds via inelastic excitations both at the molecular centre or at a ~10 nm distance after injecting hot electrons remotely. We observed that dehydrogenation always take place sequentially in adjacent arms of the molecule. We further characterized the electronic structure of fully dehydrogenated single molecules (PSM-4H) using a combination of atomic force microscopy (AFM), scanning tunnelling microscopy (STM) and spectroscopy.

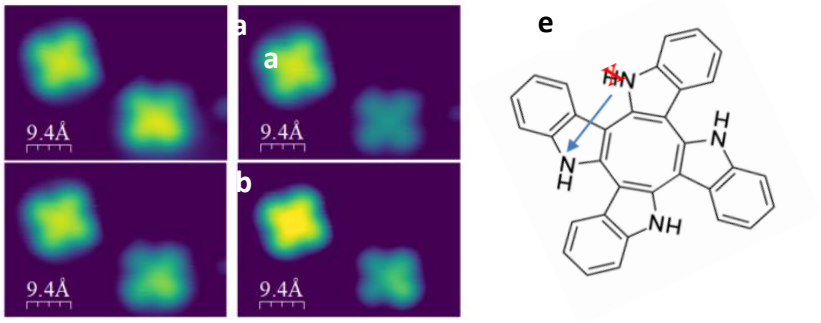

Figure 1*:* (**a-d**) STM image (V= -80mV, I=30pA) shows the sequential dehydrogenation in propeller shape molecule. (**e**) Schematic representation of the sequential dehydrogenation occurring in these molecules on the three noble metal substrates.

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Designing highly delocalized solitons by harnessing the structural parity of π-conjugated polymers

Kalyan Biswas [a,e], Jesús Janeiro [b], Aurelio Gallardo [a,c], Marco Lozano [c], Ana Barragán [a], Berta Álvarez [b], Diego Soler-Polo [c], Oleksandr Stetsovych [c], Andrés Pinar Solé [c], Koen Lauwaet [a], José M. Gallego [d], Dolores Pérez [b], Rodolfo Miranda [a], José I. Urgel [a], Pavel Jelínek [c], Diego Peña [b,] David Écija [a]

[a] IMDEA Nanoscience, 28049 Madrid, Spain
[b] CIQUS and Facultad de Química, E-15782 Santiago de Compostela, Spain
[c] Institute of Physics of the Czech Academy of Science, CZ-16253 Praha, Czech Republic
[d] Instituto de Ciencia de Materiales de Madrid (ICMM), CSIC, Cantoblanco, 28049 Madrid, Spain
[e] CIC nanoGUNE-BRTA, 20018 Donostia-San Sebastián, Spain

* k.biswas@nanogune.eu

Modern organic optoelectronics and spintronics heavily rely on π-conjugated polymers. Current efforts are directed towards designing new polymers with controlled morphology and improved electrical conductivity. One unexplored avenue involves investigating how to chemically design a π-conjugated polymer capable of hosting intrinsic solitons without relying on external doping.[1,2] In the realm of cutting-edge materials science, on-surface techniques have recently emerged as a powerful tool for crafting π-conjugated nanomaterials with unparalleled precision and previously inaccessible. Aligning with this chemical methodology and addressing a pressing challenge, we unveil an unprecedented chemical reaction based on the regio- and stereo-selective coupling of indenyl moieties. This reaction serves as the foundation for fabricating π-conjugated acenoindenylidene polymers on the Au(111) surface, featuring a longitudinal polyacetylene backbone poised to host highly dispersed solitons. Importantly, we address a crucial aspect of polymer design that has been unintentionally disregarded in experimental contexts—specifically, the role of structural parity, a fundamental factor influencing the emergence of solitons. By harnessing state-of-the-art high-resolution scanning probe microscopy and theoretical analysis, we draw a direct correlation between the structural parity of the designed polymers and their electronic properties. Notably, our investigations reveal that polymers with an odd number of units exhibit an in-gap soliton state. Thanks to their low bandgaps, these solitons extend spatially for several nanometers along the polyacetylene backbone. Our breakthroughs advance the development of π-conjugated polymers hosting dispersed quasiparticles, while circumventing the need for traditional doping through the strategic exploitation of structural parity in chemical design.

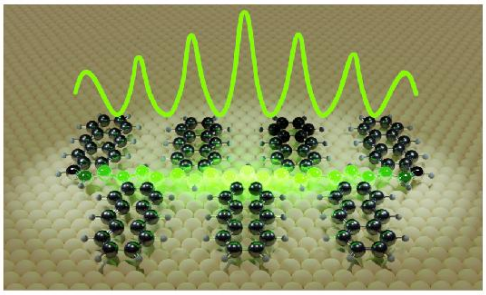

Figure - Delocalization of a soliton in a π-conjugated polymer simply by chemical design.

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Abstracts: Poster presentations

Unexpected 4x4 charge density wave in 1H-$NbTe_2$ monolayer

Noor ul Ain Iqbal[a], Jose Angel Silva-Guillén[a], Fabian Calleja[a], A. L. Vázquez de Parga[a,b,c,d], Rodolfo Miranda[a,d], Enric Carnadell[e], Miguel Angel Valbuena[a], Manuela Garnica[a,d]

[a] Instituto Madrileño de Estudios Avanzados en Nanociencia, 28049 Madrid, Spain
[b] Departamento de Física de la Materia Condensada, UAM, 28049 Madrid, Spain
[c] Condensed Matter Physics Center (IFIMAC), UAM, 28049 Madrid, Spain
[d] Instituto "Nicolás Cabrera", UAM, 28049 Madrid, Spain
[e]Institut de Ciència de Materials de Barcelona, ICMAB-CSIC, Campus UAB, 08193 Bellaterra, Spain

* noorul.ain@imdea.org

Bulk $NbTe_2$ exhibits the coexistence of charge-density wave (CDW) order and superconductivity at low temperatures. Unlike other Nb-based transition metal dichalcogenides (TMDs), which typically crystallize in the 2H phase, bulk $NbTe_2$ adopts a 1T structure. At the two-dimensional (2D) regime, $NbTe_2$ has remained elusive among Nb compounds. Recent advances in growth techniques, have enabled the epitaxial synthesis of monolayer $NbTe_2$ on gr/SiC, allowing the engineering of multiple CDW phases within its octahedral (1T) structure [1].

In this work, we report the first successful growth of 2D islands of the metastable 1H-$NbTe_2$ phase via molecular beam epitaxy on epitaxial graphene on Ir(111). This phase is identified based on its hexagonal crystal structure, distinctive spectroscopic features, and the presence of mirror twin boundaries (MTBs). Scanning tunneling spectroscopy (STS) measurements show excellent agreement with the electronic band structure obtained from angle-resolved photoemission spectroscopy (ARPES) and density functional theory (DFT) calculations, confirming the phase's stability and metallic nature. At low temperatures, STS reveals the formation of a 4x4 CDW phase. Since the 1H phase has been theoretically predicted to exhibit ferromagnetism, our results establish a promising platform to explore the interplay between magnetism and CDWs in $NbTe_2$.

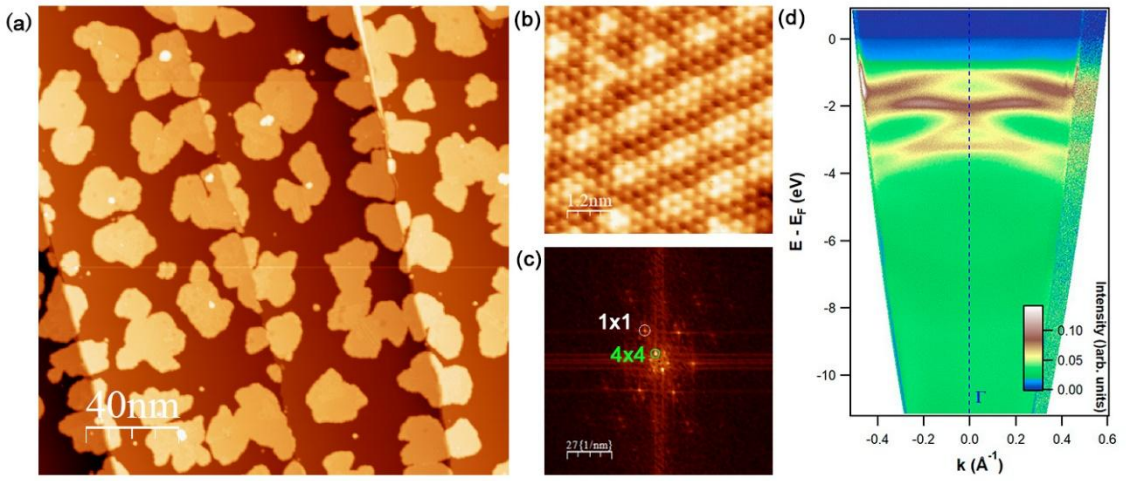

Figure - (a) Large STM image where 55% of the sample is covered with $NbTe_2$ islands (V_b=1V, I_t=100 pA, 4,6 K). (b) High resolution image and its corresponding fast Fourier transformation (FTT) (c) of the most predominant phase of $NbTe_2$ were a 4x4 CDW is observed. (V_b=-0.1V, I_t=300 pA, 4.6 K). Measurements at T = 4.2 K. (d) Band dispersion around Γ measured by ARPES at room temperature and hν = 21.2 eV.

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Tapping-mode atomic force microscopy with high-order eigenmodes for true-molecular resolution in organic thin films

R. Arilla, E. Barrena, C. Ocal, D. Martin-Jimenez

Institut de Ciència de Materials de Barcelona (ICMAB), CSIC, Campus Bellaterra 08193, Barcelona, Spain

* rarilla@icmab.es

Atomic Force Microscopy (AFM) has emerged as a powerful technique for the precise characterization of organic thin films, which serve as active layers in the development of electronic and optoelectronic devices. Typically, these characterizations are carried out under the same environmental conditions in which the devices operate—namely, ambient or low relative humidity. However, such conditions introduce an attractive force between the AFM tip and the sample prior to contact, which, in tapping mode, hinders the acquisition of molecular-resolution images. To overcome this limitation, we employ higher-order flexural eigenmodes of the AFM cantilever. These eigenmodes exhibit increased effective stiffness, enabling more stable operation in the repulsive regime with subnanometer oscillation amplitudes [1]. To evaluate the enhancement in imaging resolution as a function of the sensor's eigenmode, we conducted simulations using a point-mass model. We compared the performance of the first three flexural eigenmodes in reaching the repulsive regime under varying oscillation amplitudes and tip radii. Finally, we validated our findings by capturing AFM images of N,N-dioctyl-3,4,9,10-perylene tetracarboxylic diimide films containing individual defects, using the third flexural eigenmode. The results of this work provide an understanding of the exceptional capability of higher-order flexural modes to achieve true molecular resolution, with experimental demonstration in organic thin films.

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VS_2 Epitaxy on Strained and Relaxed Graphene

C. G. Ayani[a*], K. Kasputić[a], M. Brezak[a], Š. Mandić[a], I. Šrut Rakić[a], I. Delač[a]

[a]*Center for Advanced Laser Techniques, Institute of Physics, Bijenička Cesta 46, 10000 Zagreb, Croatia*

* cgonzalezayani@ifs.hr

Among transition metal dichalcogenides, VS_2 stands out for its theoretically predicted magnetic and strongly correlated ground states in the monolayer limit. Yet, when grown on Au(111) [1] and gr/Ir(111) [2], no net magnetization has been detected, leading to the prevailing view that the ferromagnetic ground state is not realized in pristine monolayers [2].

One possible route to alter this ground state involves tuning the material's delicate interactions—strain being a widely explored strategy. In this study, we grow VS_2 by electron beam epitaxy and investigate it using variable-temperature STM on two substrates: gr/Ir(111) as a reference [2], and strained graphene on Ir(332), a vicinal surface. Graphene grown on Ir(332) is known to experience both tensile and compressive strain depending on whether it spans terraces or step edges [3].

Our results show that VS_2 forms epitaxial islands across both regions, displaying noticeable bending (panel a). Moreover, the characteristic charge density wave (panel b) is modulated by an additional superstructure arising from the step-induced strain. These findings suggest that growing VS_2 on strained graphene/Ir(332) is a viable strategy for tuning its intrinsic ground-state properties.

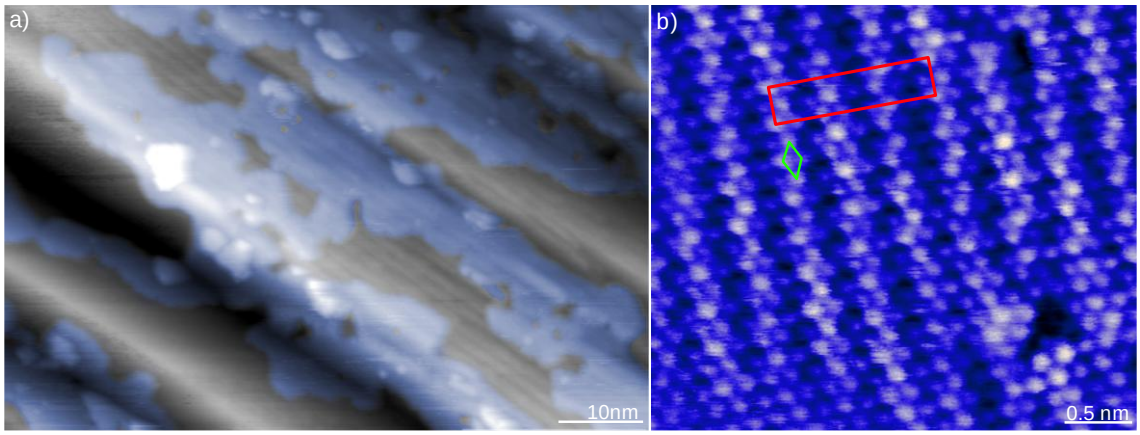

***Figure: VS_2-gr/Ir(332)**. **a)** STM image of VS_2 single layer islands, highlighted in blue, bending over the stepped areas of the gr/Ir(332) sample. Image parameters: V=750 mV, I=800 pA. **b)** Atomic resolution and charge density wave (CDW) periodicities observed over the surface of a VS_2 single layer island, the unit cells are highlighted in green and red respectively. Image parameters: V=5 mV, I=3.2 nA. T=RT.*

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Physisorption or chemisorption: unveiling the nature of functionalized MoS_2

J. Azpeitia[1], J. Mendieta-Moreno[1], L. León-Boigues[1], M. García-Hernández[1], J. A. Martín-Gago[1], C. Munuera[1], I. Palacio[1]

[1]*Instituto de Ciencia de Materiales de Madrid, CSIC, Sor Juana Inés de la Cruz 3, Cantoblanco, 28049 Madrid, Spain.*

* jon.azpeitia@icmm.csic.es

The modification of the intrinsic properties of TMDs is fundamental for achieving wider potential applications in emerging technologies. Several methods have been proposed for the effective functionalization of different TMDs normally by using their intrinsic defects present on the surface as reactive sites [1]. However, the covalent nature of the bonds between the surface and the organic linkers is still controversial [2]. In this work, we present an exhaustive study of the functionalization of MoS_2 by physical vapor deposition of thiol-containing organic molecules in ultra-high vacuum conditions. We employ 4-aminothiophenol (4-ATP) molecules to observe whether sulfur-molybdenum coordination takes place in the intrinsic sulfur vacancies of the surface. We have examined, by STM and AFM, the interaction of the 4-ATP molecule, both with the intrinsic defects present in MoS_2, and with additional defects generated by ion bombardment. In both cases, molecules present high mobility and diffusion across the sample. Additionally, we observed the release of the molecules from the surface due to interactions with the local AFM probe. Molecules attached to the probe lead to a negative contrast in the image, and therefore, molecules that appeared as bright protrusions turn into dark depressions, as shown in Figure 1. X-Ray Photoemission Spectroscopy (XPS) shows no chemical modification upon exposure, which reinforces the conclusion that molecules are adsorbed under weak electrostatic forces rather than forming covalent bonds with the MoS_2 surface.

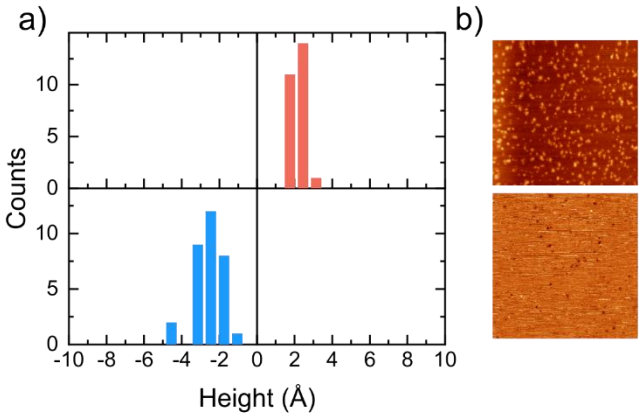

Figure 1. a) Histograms of the height distributions of the molecules on MoS_2 collected by AFM. The upper panel shows positive heights whereas the lower panel shows negative heights obtained after molecules get attached to the tip. b) Representative AFM images where molecules appear as bright and dark features.

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Nano-surface photovoltage study of halide perovskite solar cells

Parmenio Boronat Sevilla[a], Omar E. Solis[a], Ana Cros[a], Pablo P. Boix[a,b], Núria Garro[a]

[a] Institut de Ciència dels Materials de la Universitat de València (ICMUV), València, Spain
[b] Instituto de Tecnología Química (ITQ, CSIC), València, Spain

* parmenio.boronat@uv.es

Scanning probe microscopy can unveil many physical processes that still hinder the efficiency and stability of solar cells based on halide perovskites (HaP). For instance, there is still an open debate on whether grain boundaries related to polycrystalline growth are beneficial or detrimental to the overall HaP solar cell operation. To resolve this issue, establishing a clear correlation between nanoscale morphology and optoelectronic properties is essential. Another intricated challenge is the efficiency of electron/hole extraction at the interfaces between the HaP and the transport materials (ETL/HTL) which is affected by charge recombination, trapping and ion migration. Among HTLs, organic materials are easier to prepare but can also degrade under operation conditions. Here Kelvin probe force microscopy (KPFM) can be used to map the surface photovoltage (SPV) of the buried interface and its evolution with time [1].

In this work, we aim to grant an insight on how both micro and macro properties can be combined to attain a whole description of HaP solar cell devices. To do so, half-cells consisting of polycrystalline methyl-ammonium lead iodide (MAPI) deposited on top of different organic HTL materials (PEDOT:PSS, PTAA, 2PAC) have been mapped by light-assisted KPFM and conductive AFM. Conductivity maps (Fig. 1a) and I-V curves at different grains have also provided relevant information to understand the role of grain boundaries in charge transport and local current losses. SPV transients (Fig 1b) have been correlated with charge trapping and ionic migration at the interfaces, both affecting the stability of the device. . The power dependence of SPV (Fig 1c) has been used to determine the ideality factor (η) of the junction and to study its variation with excitation wavelength and the exposure to ambient conditions.

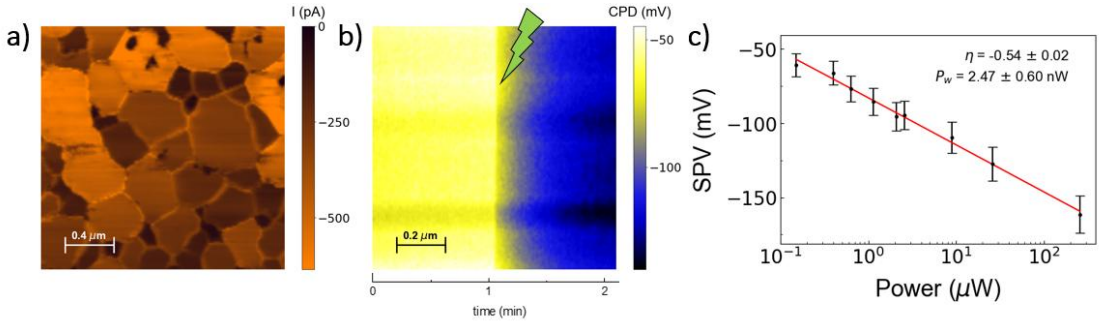

Figure 1: Characterization of a MAPI-2PAC half-cell device. a) Conductivity map at -0.5 V. b) One-line light-assisted KPFM map showing the transient evolution of SPV of different grains.. C) Logarithmic SPVpower dependence is fitted to obain the ideality factor [2].

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Co-localized KPFM & Raman scattering studies of graphene oxide reduction

V. Camús [a]*, M. Navarro-Rodríguez [b], N. Garro [a], A. Cros [a], E. Palacios-Lidón [b]

[a] Universitat de València, Institut de Ciència dels Materials (ICMUV), Paterna, 46980, València, Spain

[b] Universidad de Murcia, Centro de Investigación en Optica y Nanofisica (CIOyN), Murcia, 30100, Murcia, Spain

* victor.camus@uv.es

Graphene oxide (GO) is a graphene-derived 2D material characterized by a defective carbon basal plane randomly decorated with oxygen-containing functional groups, such as epoxides, hydroxyls, and carboxyls. These functional groups disrupt the sp^2 carbon network, rendering GO electrically insulating, highly disordered, and hydrophilic, while also making it soluble in polar solvents. The reduction of GO, through either chemical or thermal methods, removes a significant portion of these oxygen groups, yielding reduced graphene oxide (rGO). This process restores the sp^2 carbon network to varying degrees, resulting in a material with improved electrical conductivity, hydrophobicity, and insolubility in polar solvents. However, the reduction process often introduces structural defects and heterogeneity, which can significantly influence the material's properties. [1]

In this work, we present a detailed investigation of the local reduction degree, nanoscale electronic properties, chemical composition, and structural defects of GO and rGO samples prepared via both chemical and thermal reduction methods. To achieve this, we employ a co-localized approach combining Kelvin Probe Force Microscopy (KPFM), Raman spectroscopy and Tip Enhanced Raman Scattering (TERS). The combined application of theses techniques allows us to correlate the local electronic properties with the chemical and structural characteristics of rGO at the nanoscale.

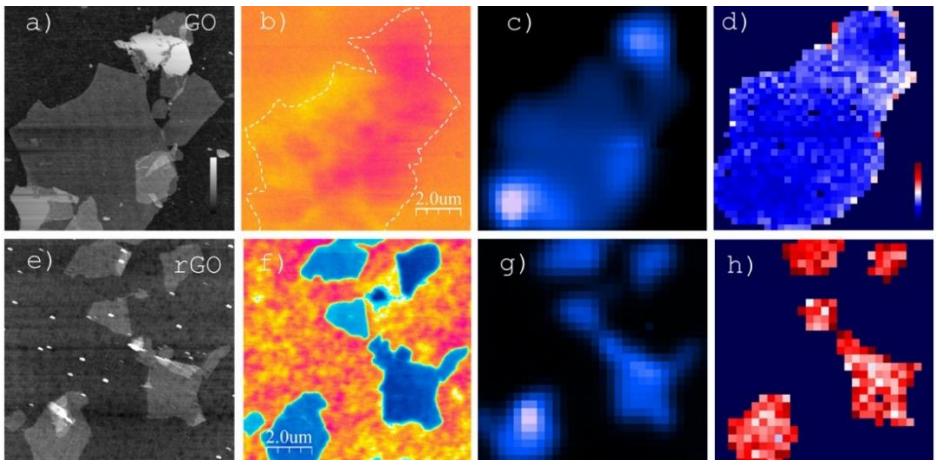

Figure - Co-localized KPFM-Raman scattering maps corresponding to GO and chemically reduced rGO flakes. For GO: (a) topography; (b) SP; (c) integrated Raman intensity; (d) ID∗⁄IG ratio. For rGO: (e) topography; (f) SP; (g) integrated Raman intensity; (h) ID∗⁄IG ratio. z scales are: 10 nm for topography; 200 mV for SP; 12 000 arbitrary units for Raman intensity; and 0.2 for D∗⁄G intensity ratio. [2]

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Twistraintronics: mechanical and electronic *in-situ* manipulation of magic angle graphene using STM

R. Carrasco [a,b], F. Escudero [c,d], Z. Zhan [d], P.A. Pantaleon [d], F. Guinea [d,e,f] and I. Brihuega [a,b]

[a] Departamento Física de la Materia Condensada, Universidad Autónoma de Madrid, Madrid E-28049, Spain
[b] Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid Madrid E-28049, Spain
[c] IFISUR, Departamento de Física, CONICET, Universidad Nacional del Sur, Av. Alem 1253, B8000 Bahía Blanca, Argentina
[d] IMDEA Nanoscience, Faraday 9, 28049 Madrid, Spain
[e] Donostia International Physics Center, Paseo Manuel de Lardizábal 4, 20018 San Sebastián, Spain
[f] Ikerbasque, Basque Foundation for Science, 48009 Bilbao, Spain

* roberto.carrasco@uam.es

Stacking layers of 2D materials with a certain twist angle creates moiré superlattices that fundamentally alter electronic structure and interactions, giving rise to exotic properties [1] such as correlated insulating states, unconventional superconductivity, and topological phases. However, robust van der Waals interactions make it difficult to modify the twist angle once the layers are stacked, limiting tunability after assembly. Strain offers a complementary approach, capable of modifying electronic structure [2,3] in a similar way to twist, while providing greater flexibility for *in situ* tuning. Here, we demonstrate control of local strain on graphene by visibly changing magic-angle moiré from trigonal to square pattern by manipulating graphene wrinkles [4] using STM. STS measurements confirm that this structural manipulation is accompanied by significant electronic modifications. We show that the observed electronic modifications can be accurately described by a continuum model incorporating shear strain and a Hartree potential, directly altering the local density of states and band structure. Our findings establish strain as a powerful and tunable parameter for engineering moiré superlattices, paving the way for new strategies to control electronic properties in twisted 2D materials.

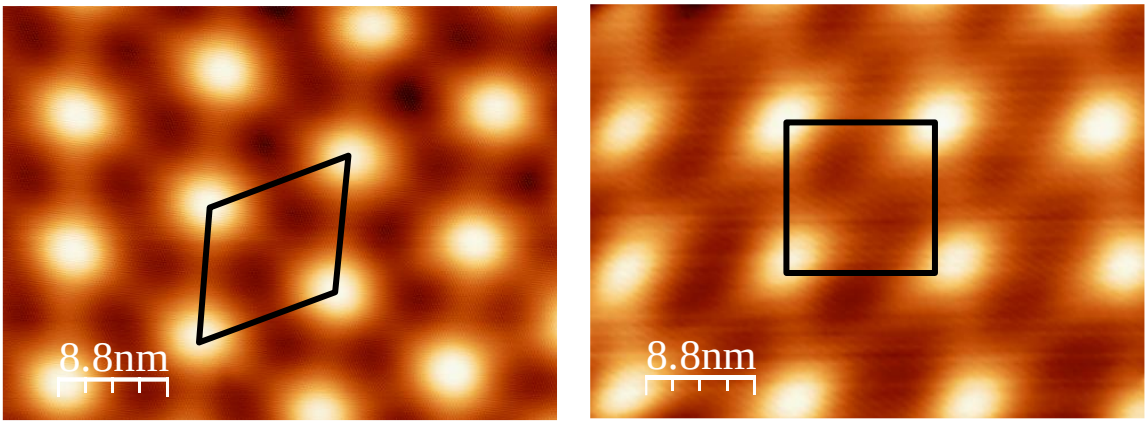

Figure – STM images of graphene moiré superlattices, showing a strain-induced transition. To the left, a trigonal magic-angle moiré pattern arising solely from twist. To the right, a square magic-angle moiré resulting from both twist and strain simultaneously.

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Polar Crystalline order on asymmetric BTBT Derivatives revealed by Kelvin Probe Force Microscopy

Alba Cazorla [a], Shunya Yan [a], Eduardo Solano [b], Daniel Martin [a], Esther Barrena [a]

[a] Instituto de Ciencias de Materiales de Barcelona (ICMAB-CSIC)
[b] Sincrotrón ALBA

* acazorla@icmab.es

Understanding the structure and polymorphism of organic electronic materials is essential for optimizing device performance. A key example is 7-decyl-2-phenyl[1]benzothieno[3,2-b][1]-benzothiophene (Ph-BTBT-10), where high charge carrier mobility is related to a structural transformation from a metastable thin-film phase to a stable bilayer phase with a head-to-head configuration [1]. Such configuration cancels the intrinsic longitudinal electric dipole moment that results from the asymmetric molecular structure.

Remarkably, using Kelvin Probe Force Microscopy (KPFM), we have demonstrated the formation of a polar polymorph in thin films of Ph-BTBT-10, driven by the growth of a layered stacking with unidirectionally oriented molecules [2,3]. Our previous work highlighted KPFM as a powerful tool for detecting polar order and tracking temperature-induced structural transitions.

In this work we have expanded our investigation to other asymmetric BTBT derivatives with a varying length of the side alkyl chain (n=4,8,10,12) employing a combination of both KPFM and Grazing Incidence Wide Angle X-ray Scattering (GIWAXS). This study examines systematically the effect that the variation of the molecular dipole moment has on the formation of crystalline polar structures. Their stability with thermal annealing is monitored *in situ* by KPFM and further correlated with GIWAXS experiments.

The findings emphasize the crucial role of polar polymorphs at the dielectric interface and their direct impact on the performance of organic field-effect transistors (OFETs). Ultimately, achieving isotropic thin films with minimal electrostatic disorder is essential for the optimal design and enhancement of high-performance OFETs.

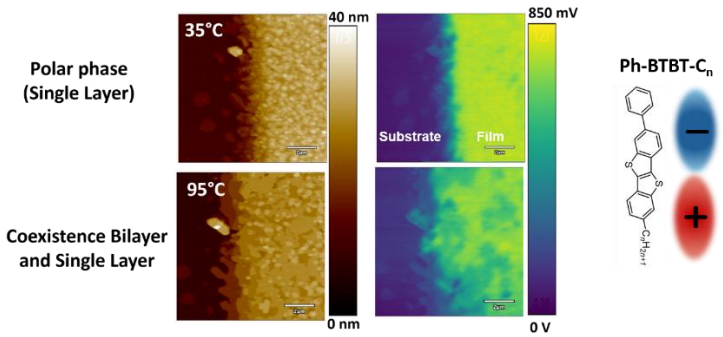

Figure – Topography images (left) with their corresponding surface potential maps (middle) for 20 nm sample of Ph-BTBT-8 at 35ºC (top) and at 95ºC (bottom). Right part: Chemical structure of Ph-BTBT-Cn derivatives with scheme of their electrostatic distribution.

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Torsional Mode Dynamic AFM as versatile multifrequency mode: challenges and possibilities

J. Colchero [a *], Giovanni Sáenz-Arce [a,b]

[a] CIOyN, Dept. Física, Campus Espinardo, Universidad de Murcia, Murcia, Spain.
[b] Facultad de Ciencias Exactas y Naturales, Universidad Nacional, Heredia 86-3000, Costa Rica.

* colchero@um.es

A novel dynamic Atomic Force Microscopy (DAFM) has become a versatile tool in Nanoscience due to its ability to measure not only nanoscale topography, but also a variety of surface properties; in particular electrostatic and magnetic behavior, as well as nanoscale wetting behavior -to name only a few- can be inferred by appropriate analysis of tip-sample interaction. Generally, in DAFM the tip is oscillated in a direction normal to the sample surface, allowing to measure the Force Gradient F′(z) of tip-sample interaction in this direction, as well as dissipative processed related to the motion normal to the surface (typically “z-direction”). If the tip is oscillated laterally -so called “torsional mode”, it should be possible to determine lateral force gradients, and dissipation associated with lateral displacements. While this mode has been proposed quite long ago, it seems surprising that up to now it is used rather little.

We believe that one problem associated with lateral/torsional oscillation is related to the calibration of oscillation amplitude. In this work we will show that accurate calibration of oscillation amplitude in torsional mode is crucial for the correct analysis and interpretation of data in experiments involving dynamic in scanning force microscopy. In fact, surprisingly this mode has a quite high sensitivity (in our case close to 1pm!), which may be detrimental for typical imaging applications, since very large lateral oscillations may be induced, resulting in uncontrolled imaging conditions.

This study focuses on the development and implementation of advanced methods to calibrate the oscillation amplitude in systems operating in torsional mode. A combination of theoretical and experimental approaches is employed to enhance the accuracy and repeatability of oscillation measurements. The typical electronics used to process the dynamic motion of the cantilever can be adjusted to transfer the thermal noise of the cantilever motion from its resonance frequency to a much lower frequency within the typical bandwidth of the corresponding data acquisition electronics of a scanning force microscopy system. The applications of this enhanced calibration method are far-reaching, particularly in the study of liquid neck formation and rupture. Accurate measurements of torsional oscillations are essential for understanding the dynamics of liquid bridges and the forces involved in their stability and breakage. The advancements proposed have significant implications for the accurate measurement of dynamic processes, with specific applications in the formation and rupture of liquid necks, thus contributing to the broader field of material science and nanotechnology in wetting properties of surface.

New insights into tobacco mosaic virus: stability, disassembly and uncoating

Alejandro Díez-Martínez [a,b], Pablo Ibáñez-Freire [a,b], Diego Alonso Aldave [a,b], Salvatore Assenza [a,b], David Reguera[c], Pablo Ares [a,b], Julio Gómez-Herrero [a,b], Alexander Bittner [d] and **Pedro J. de Pablo** [a,b]

[a] Department of Condensed Matter Physics, Universidad Autónoma de Madrid, Spain.
[b] Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, Madrid, Spain.
[c]Departament de Física de la Matèria Condensada, Universitat de Barcelona, Barcelona, Spain.
[d] CIC nanoGUNE Consolider, Donostia-San Sebastián, Spain.
Email: (p.j.depablo@uam.es)

Tobacco mosaic virus (TMV) serves as a key model in both virology and nanotechnology, admired for its robust structure and ease of assembly. While the mechanical resistance of TMV has attracted interest for nanostructure applications [1], the intricate details of its disassembly mechanics remain poorly understood. In this study, we integrate three key aspects of TMV behavior: its mechanical resilience, its thermal stability and the role of genome-protein interactions. By combining nanoindentation experiments with coarse-grain and finite elements simulations [2], we investigate how the viral capsid disassembles as a function of the force applied. Which reveals that the central cavity plays a critical role in the distribution of mechanical stress [3]. We also heated TMV up to 175ºC and found almost no structural degradation. Beyond this temperature, its height follows a sigmoidal curve until its complete degradation at 250ºC. Additionally, we explore how the specific nucleotide sequence of the TMV RNA affects the weakening of specific regions during mechanical disassembly [4]. Using Atomic Force Microscopy (AFM), we correlate the formation of rifts along the capsid with the trimers in the genomic sequence, shedding light on how these interactions contribute to the mechanical stability of the virus. Together, this combined approach provides a deeper understanding of the structural integrity of TMV and the factors that govern its disassembly process.

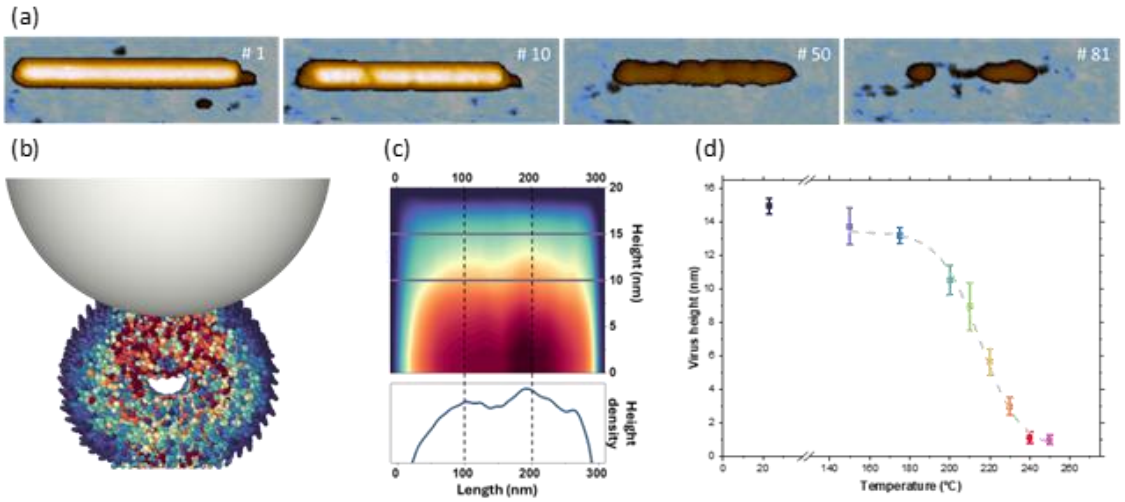

Figure –(a) Mechanical fatigue on TMV particle: #1 first frame, #10 beginning of disassembly, #50 disappearance of the upper half, and #81 final remains. (b) Coarse grain simulation of an indentation showing an uneven mechanical stress distribution. (c) TMV average disassembly pattern. (d) Distribution of TMV heights at different temperatures

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Generating antiaromaticity in polycyclic conjugated hydrocarbons by thermally selective skeletal rearrangements at interfaces

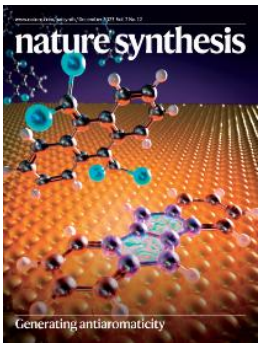
E. Pérez-Elvira[a], A. Barragán[a], Q. Chen[b], D. Soler-Polo[b], A. Sánchez-Grande[a,c], D. J. Vicent[c], K. Lauwaet[a], J. Santos[c], P. Mutombo[b], J. I. Mendieta-Moreno[b], B. de la Torre[d,e], J. M. Gallego[a,f], R. Miranda[a], N. Martín[a,c], P. Jelínek[b,g], J. I Urgel[a], and **D. Écija[a,*]**

* david.ecija@gmail.com

[a]IMDEA Nanoscience, Campus de Cantoblanco, Madrid, Spain.
[b]Institute of Physics of the Czech Academy of Science, Praha, Czech Republic.
[c]Departamento de Química Orgánica, Facultad de Ciencias Químicas, Universidad Complutense de Madrid, Madrid, Spain.
[d]Faculty of Mathematics and Physics, Charles University, Praha, Czech Republic.
[e]Nanomaterials and Nanotechnology Research Center (CINN) CSIC-UNIOVI-PA, 33940 El Entrego, Spain
[f]Instituto de Ciencia de Materiales de Madrid, CSIC, Cantoblanco, Madrid, Spain.
[g]Regional Centre of Advanced Technologies and Materials, Czech Advanced Technology and Research Institute (CATRIN), Palacký University Olomouc, Olomouc, Czech Republic.

Antiaromatic polycyclic conjugated hydrocarbons (PCHs) are attractive research targets because of their interesting structural, electronic and magnetic properties. Unlike aromatic compounds, the synthesis of antiaromatic PCHs is challenging because of their high reactivity and lack of stability, which stems from the small energy gap between their highest occupied and lowest unoccupied molecular orbitals.

Here we describe a strategy for the introduction of antiaromatic units in PCHs via thermally selective intra- and intermolecular ring-rearrangement reactions of dibromomethylene-functionalized molecular precursors upon sublimation on a hot Au(111) metal surface, not available in solution chemistry. The synthetic value of these reactions is proven by the integration of pentalene segments into acene-based precursors, which undergo intramolecular ring rearrangement, and the formation of π-conjugated ladder polymers, linked through cyclobutadiene connections, due to ring-rearrangement and homocoupling reactions of indenofluorene-based precursors. The reaction products are investigated by scanning tunnelling microscopy and non-contact atomic force microscopy, and mechanistic insights are unveiled by computational studies.[1]



Artistic representation of a carbon skeletal rearrangement on Au(111), incorporating antiaromatic moieties into the compound.

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A new modular Atomic Force and Optical Microscope as nanoLab

J.M. Filiu Samper [a *], M.M. Calvo Lebron [a], A. Colchero Truniger [b], J.F González Martínez [b,c], J.Colchero Paetz [a]

[a] CIOyN, Dept. Física, Campus Espinardo, Universidad de Murcia, Murcia, Spain.
[b] Department of Biomedical Science, University of Malmö, Malmö, Sweden.
[c] Departamento de Física Aplicada, Universidad Politécnica de Cartagena, Cartagena, Spain.

* josemanuel.filius@um.es

A novel AFM-optical microscope has been designed with the goal of very high stability, low thermal drift, modular design, easy access and easy integration into other experimental setups, in particular Optical Microscopy and/or Synchrotron Radiation facilities.

The fundamental design criterion has been to separate the AFM system into three different (and modular) parts, each having different requirements with respect to stability and size. First, the smallest stage integrating the AFM tip holder and sample scanner having (sub-) nanometer stability; second, the optical stage with the components for the optical lever detection scheme; and third a stage having all additional techniques to be combined with AFM measurements, which are “looking” at the same sample spot as the AFM tip. This third stage may be conceptually as large as needed. In the simplest case it will only have the components needed for optical microscopy. However, it may also be a whole optical table or even a Synchrotron radiation source.

The main challenge will be to allow for high numerical aperture access for optical characterization, in particular Raman Scattering (RS), as well as parallel/front view access for tip-enhanced RS and X-Ray-Scattering applications; while still maintaining high rigidity and low noise and low drift in AFM applications. The system will be modular using infinitely corrected objectives to have a collimated beam path that allows for high resolution optical microscopy of the tip-sample region that is being characterized also by AFM techniques. In addition to optical techniques, we aim to expand the capabilities of this modular AFM system to include X-ray Scattering (SAXS), Grazing-Incidence Small-Angle X-ray Scattering (GISAXS), and other related methodologies. The design's modularity inherently simplifies the fusion of AFM with these X-ray techniques, unlocking new possibilities for comprehensive nanoscale characterization.

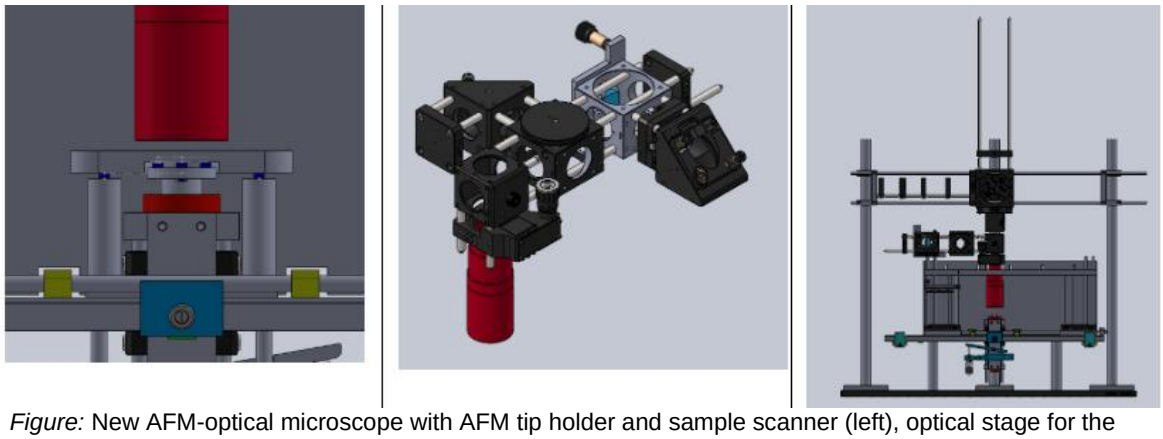

Figure: New AFM-optical microscope with AFM tip holder and sample scanner (left), optical stage for the optical lever detection (middle), and third stage with techniques to be combined with AFM.

A chemical reaction triggered on ultrashort time scales with single-molecule selectivity

Niklas Friedrich [a], Carmen Roelcke [a], Tzu-Chao Hung [a], Yaroslav Gerasimenko [a], Rupert Huber [a], Jascha Repp [a]

[a] Institute of Experimental and Applied Physics, University of Regensburg, Regensburg, Germany

* Niklas.friedrich@ur.de

In lightwave-driven scanning tunnelling microscopy (LW-STM), the electric-field transient of ultrashort laser pulses focused into the junction of a scanning tunnelling microscope acts as a voltage transient and thereby controls tunnelling on ultrashort timescales [1]. This allows unravelling the dynamics of quantum systems in pump-probe experiments with atomic spatial and femtosecond temporal resolution [2, 3].

Here, we show that LW-STM can be used to trigger chemical reactions on ultrashort timescales. We study free-base naphthalocyanine molecules (H_2Nc) on 2ML NaCl on Cu(100). In DC-biased experiments, this system switches between different tautomers upon injection of high-energy tunnelling electrons [4]. We find that the same reaction is facilitated by ultrashort voltage transients in LW-STM for transients far exceeding the voltage of the lowest unoccupied molecular orbital. Furthermore, even a stepwise deprotonation of the molecule is activated by the ultrashort laser pulses when increasing the voltage transient beyond a threshold value.

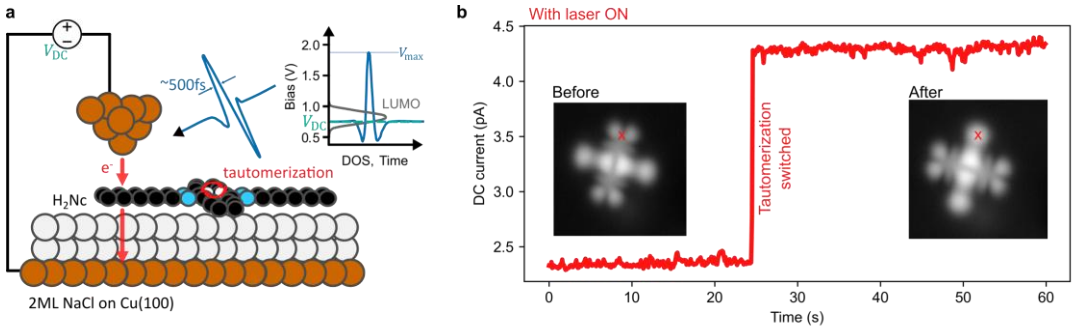

Figure – **a** Sketch of the experiment: An ultrashort THz pulse is coupled to the tip of an STM and acts as an ultrashort bias transient in the tunneling junction enabling the tunneling of high-energy electrons. These electrons can trigger switching between the two tautomers of H_2Nc positioned on 2ML NaCl on Cu(100). **b** The occurrence of the chemical reaction is monitored by the telegraph noise of the DC current when the tip is positioned over one extremity of the molecule. STM inset images ($\boldsymbol{V = 750\,mV}$, $\boldsymbol{I = 5\,pA}$) show the H_2Nc before and after the tautomerization reaction occurring at $\boldsymbol{t = 25\,s}$.

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On-Surface Synthesis of (1,3)-chGNRs with Five-Membered Ring Edge Extensions

S. Galán [a], A. Jiménez-Martín [b], A. Martínez [c], S. Salaverría [d], J. Rodríguez-Fernández [a,d], D. Peña [c,e], D. G. de Oteyza [d], B. de la Torre [b,d]

[a] Physics Department, University of Oviedo, 33007 Oviedo, Spain
[b] Regional Centre of Advanced Technologies and Materials, Czech Advanced Technology and Research Institute (CATRIN) Palacký University, Šlechtitelů 27, 78371 Olomouc, Czech Republic
[c] Center for Research in Biological Chemistry and Molecular Materials (CiQUS) and Department of Organic Chemistry, University of Santiago de Compostela, Santiago de Compostela 15782, Spain.
[d] Nanomaterials and Nanotechnology Research Center (CINN), CSIC-UNIOVI-PA, 33940 El Entrego, Spain
[e] Oportunius, Galician Innovation Agency (GAIN), 15702 Santiago de Compostela, Spain

* galansantiago@uniovi.es

Graphene nanoribbons (GNRs) exhibit highly tunable electronic properties, making them promising candidates for next-generation nanoelectronic and optoelectronic devices. Precise control over their atomic structure, including width, crystallographic symmetry, heteroatom doping, and edge termination, is crucial for tailoring their electronic behavior.

Here, we introduce a novel strategy for the edge functionalization of (3,1)-chiral graphene nanoribbons (chGNRs) by incorporating five-membered rings into their backbone. Using 2,2′-dibromo-9,9′-bianthracene precursors equipped with alkyne groups, we induce selective ethynylarene rearrangement via on-surface cycloaddition, leading to the formation of cyclopenta-fused polycyclic aromatic hydrocarbons at the nanoribbon edges. High-resolution scanning tunneling microscopy (STM) and atomic force microscopy (AFM) reveal the integration of five-membered rings in both ortho- and para- configurations, significantly modifying the chGNRs' electronic structure. This approach demonstrates a new avenue for structural and electronic engineering of GNRs.

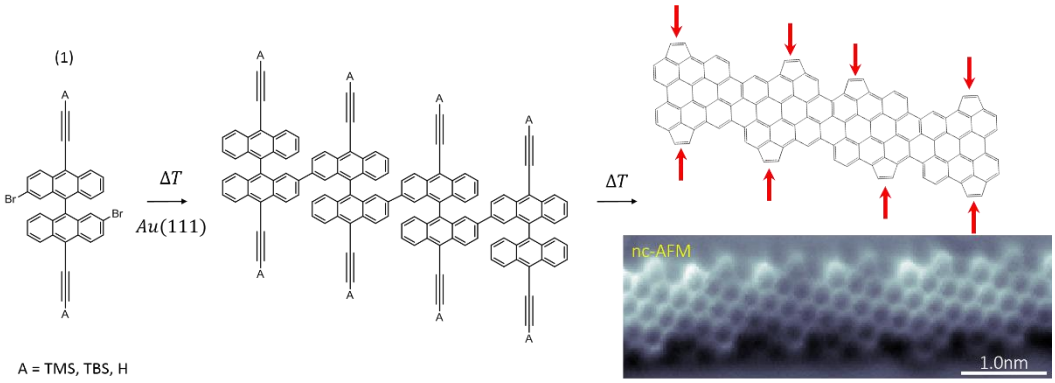

Figure – Scheme of the reaction including the molecular precursor (1), polymerization and cyclization. Constant height high-resolution nc-AFM image with a CO-decorated tip of the edge extended chiral graphene nanoribbon.

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Tailoring on-surface polymerization by molecular coverage through indenyl coupling

Alba García Frutos [a], Kalyan Biswas [a,d], Jesús Janeiro [b]Marco Lozano [c], Ana Barragán [a], Berta Álvarez [b], Diego Soler-Polo [c], Koen Lauwaet [a], José M. Gallego [a], Dolores Pérez [b], Rodolfo Miranda [b], José I. Urgel[a], Pavel Jelínek[c], Diego Peña [a,] David Écija[a]

[a] IMDEA Nanoscience, 28049 Madrid, Spain
[b] CIQUS and Facultad de Química, E-15782 Santiago de Compostela, Spain
[c] Institute of Physics of the Czech Academy of Science, CZ-16253 Praha, Czech Republic
[d] CIC nanoGUNE-BRTA, 20018 Donostia-San Sebastián, Spain

*alba.gfrutos@imdea.org

Indenyl coupling refers to the reaction where molecular precursors equipped with indenyl ligands promote the formation of C-C bonds, thanks to deprotonation of indenyl groups and subsequent homocoupling. This leads to extended π- conjugated polymers along a polyacetylene backbone, expanding the electronic delocalization, which is crucial to obtain π-conjugated systems with broad applications in fields such as spintronics, sensing, optoelectronics and photovoltaics, among others.[1]

In this work, we present an on-surface chemical reaction in ultra-high vacuum conditions based on the regio- and stereo-selective covalent coupling of indenyl moieties[1] for fabricating π-conjugated systems whose dimensionality is directly driven by the initial molecular coverage of the precursor on the surface. The deposition of a dicyclopentaanthracene species (**1**) on Au(111) and its subsequent post-annealing at 150ºC leads to the controlled formation of various π-conjugated polymers. When the coverage is low (less than 0.3 ML), 1D chains with –syn and –anti bonding connections emerge (**2**). If the molecular coverage is around 0.5 ML, 1D extended zipper-like polymers are obtained (**3**). Finally, at very high coverage (almost 1 ML), small 2D patches are observed (**4**), whose size can be promoted by long annealing. By using scanning tunneling microscopy and non-contact atomic force microscopy, complemented by density functional theory simulations, the structural and electronic properties of the distinct polymers were rationalized. Notably the termini of the polymers are always doubly-hydrogenated as displayed in Figure 1. In addition we observe bandgaps of 3,2 eV for 1, 2,03 eV eV for 2 and 3,5 eV eV for 3, respectively.

Our results open avenues for the controlled design of molecular nanoarchitectures on surfaces, while exploiting a recently discovered reaction at interfaces, the indenyl coupling.

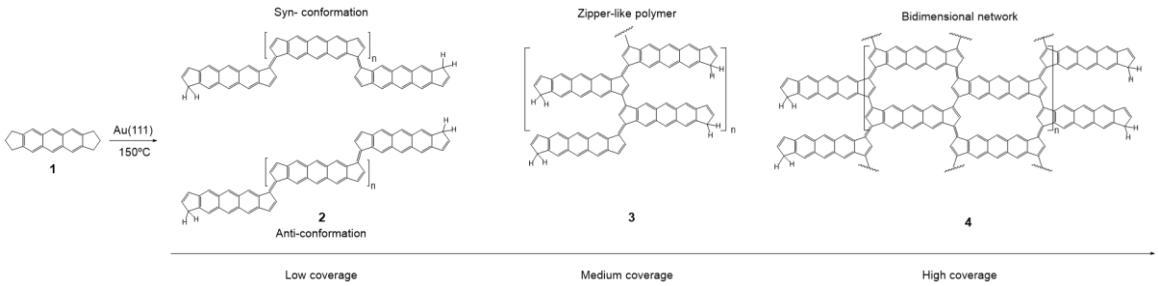

Figure 1. Dependence of the degree of polymerization on the molecular coverage.

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Magnetically induced modifications of topological surface states mediated by Rare-Earth surface doping

Beatriz Muñiz Cano[a], Fabian Calleja[a], Ji Dai[b], Massimo Tallarida[b], Vera Marinova[c], Adriana I. Figueroa[d], Kevin García-Díez[b,e], Aitor Mugarza[e,f], Sergio O. Valenzuela[e,f], Amadeo L. Vázquez de Parga[a,g], Rodolfo Miranda[a,g], Julio Camarero[a,g], Francisco Guinea[a], Jose Angel Silva-Guillén[a], **Manuela Garnica**[a] and Miguel A. Valbuena[a]

[a] IMDEA Nanociencia, 28049 Madrid, Spain.
[b] ALBA Synchrotron Light Source, 08290 Barcelona, Spain.
[c] Institute of Optical Materials and Technologies, Bulgarian Academy of Sciences, 1113 Sofia, Bulgaria
[d] Departament de Física de la Matèria Condensada, Universitat de Barcelona, Barcelona, Spain.
[e] Catalan Institute of Nanoscience and Nanotechnology (ICN2), Barcelona, Spain
[f] ICREA Institució Catalana de Recerca i Estudis Avançats, 08010 Barcelona, Spain.
[g] Departamento de Física de la Materia Condensada, Instituto "Nicolás Cabrera" and Condensed Matter Physics Center (IFIMAC),UAM, 28049 Madrid, Spain.
* manuela.garnica@imdea.org

Magnetic topological insulators (MTIs) are a unique class of materials where the coexistence of a topologically protected band structure with long-range ferromagnetic order can break time-reversal symmetry (TRS). This symmetry breaking introduces a bandgap in the Dirac cone-shaped topological surface state (TSS), a prerequisite for realizing the quantum anomalous Hall effect (QAHE). The QAHE, characterized by dissipationless, spin-polarized edge currents, offers promising applications in spintronic devices but remains challenging to achieve experimentally, especially at practical temperature conditions [1].

In this study, we investigate the effects of Er doping on Bi_2Te_3, a prototypical three-dimensional topological insulator. Using angle-resolved photoemission spectroscopy (ARPES) and scanning tunneling microscopy (STM), we explore how Er surface doping influences the TSS. Bi_2Te_3 exhibits a strongly warped Fermi surface [2], and Er doping leads to distinct modifications of the TSS, further highlighting the substrate-dependent nature of these interactions. After a controlled Er evaporation, STM reveals the formation of small hexagonal islands along with atomic defects on the Bi_2Te_3 surface. Additionally, fast Fourier transform (FFT) analysis of quasiparticle interference (QPI) maps is compatible with a triangular energy contour in agreement with ARPES. These results provide further insight into the interaction between Er and the TSS, reinforcing the potential for tuning magnetic properties and band structure in MTIs. Our findings open a viable pathway toward achieving the QAHE and integrating MTIs into spintronic technologies.

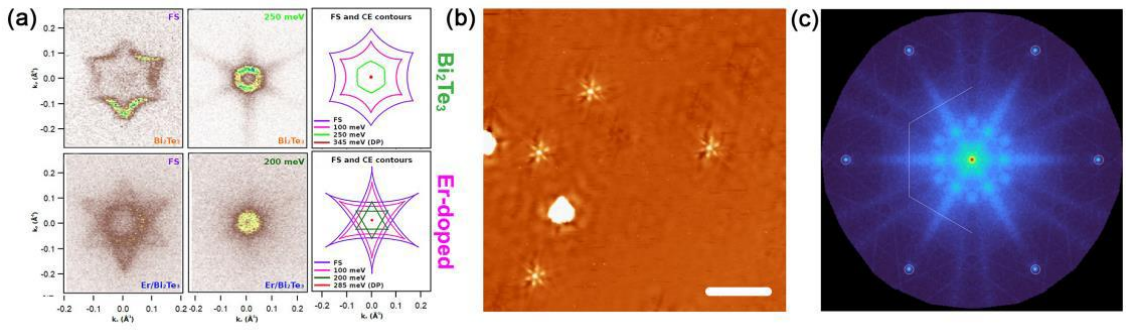

Figure - (a) Experimental FS and CE map at 250 meV, along with contours derived from the curvature maps of the raw data at different energies for pristine Bi2Te3 and Er-doped Bi2Te3. (b) dI/dV map of a Bi2Te3 surface after Er deposition (0.5V, 1nA, scale bar 8 nm) (c) Symmetrized Fourier transformed image of a dI/dV map at 400 meV

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On-surface-synthesis of atomically precise hybrid graphene nanoarchitectures

P. González-Izquierdo [a], M. Barquín [a], I. Hernández Campo [a], M. N. Sanz-Ortiz [a], M. de Pedro del Valle [a], C. Moreno [a]

[a] Departamento de Ciencias de la Tierra y Física de la Materia Condensada, Universidad de Cantabria, 39005 Santander, Spain

*palmerina.gonzalez@unican.es

We present the synthesis of two 2D organometallic nanostructures, following a two-step OSS strategy developed previously to obtain long-range order nanoporous graphene (NPG) [1], doped/undoped lateral heterostructures of GNRs [2] and quantum tunable molecular-bridged GNRs [3]. First, molecular precursors were evaporated onto a Au(111) substrate and annealed to induce polymerization and subsequent planarization to form GNRs via a surface-assisted reaction. This pre-aligned GNR array serves as a template for the second step, where the spin-bearer molecules (Bis(Dithiobenzil) Nickel and Vanadium(IV) oxide meso-tetraphenylporphine) were deposited and subsequently annealed to promote lateral bonding. STM imaging reveals the formation of a laterally extended hybrid network, while STS measurements provide insight into the electronic density of states. Additionally, we transferred the hybrid graphene nanostructures to a Si/SiO_2 substrate, a key step for their integration in real devices. The success of the transfer was assessed through Raman spectroscopy.

This work demonstrates the feasibility of using OSS to fabricate hybrid graphene nanoarchitectures with embedded transition metal centers, by using periodically ordered GNRs as a 2D scaffold.

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Imaging noise in non-contact Dynamic Atomic Force Microscopy

J.F. González Martínez [a], J. Colchero [b]

[a] Departamento de Física Aplicada, Universidad Politécnica de Cartagena, Cartagena, Spain.
[b] CIOyN, Dept. Física, Campus Espinardo, Universidad de Murcia, Murcia, Spain.

* juanf.gonzalez@upct.es

From a fundamental point of view, generally either statistical or quantum noise limits the ultimate resolution. In the first case (statistical or "thermal" noise), according to the dissipation-fluctuation theorem, noise is related to the dissipation within a physical system. The second case, measurements at the quantum limit [1], is receiving increased interest also in the AFM community. In the present work, we measure and discuss noise in the tip-sample interaction for non-contact Dynamic Atomic Force Microscopy (nc-DAFM). We discuss how thermal noise allows to precisely calibrate the oscillation amplitude in Dynamic SFM [1]; and that it is possible to acquire "noise" images showing a well-defined pattern (Figure 1, [4]), different from topography or other acquisition channels. This noise is attributed to the interaction induced by liquid necks forming between tip and sample [3]. While previous analyses identified thermal noise as the dominant contribution to frequency fluctuations, experimental evidence reveals the presence of this additional, significantly stronger noise source when tip–sample interactions are present. This interaction-induced noise carries valuable information about the chemical nature of the sample, turning what is conventionally regarded as a limiting factor into a rich signal.

We discuss how a typical nc-DAFM can be adjusted to transfer noise of the cantilever motion from its resonance frequency to a much lower frequency within the typical bandwidth of the corresponding electronics [2]. For typical applications thermal noise is generally considered the most important noise source in a SFM setup. Here we show however that additional noise sources may be present in Dynamic SFM measurements [4], which may be significantly larger than thermal noise. Using different SFM techniques (Force Spectroscopy, Kelvin Probe Microscopy, 3D modes, etc), we analyze this noise for amphiphilic molecules (SDS) adsorbed on a graphite substrate. Our experiments show that the different chemical nature of these materials induce a different magnitude of the measured noise, leading to an image with "chemical" contrast (Figure 1).

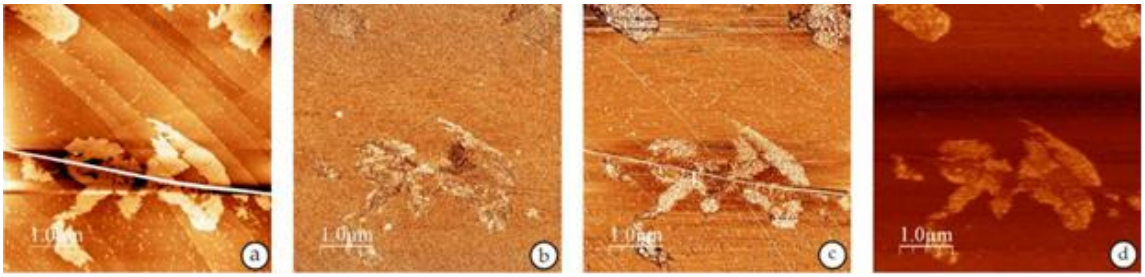

Figure - Topography (a), frequency shift (b), contact potential (c) and noise images (d) acquired simultaneously in nc-DAFM (topography feedback performed at constant oscillation amplitude).

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Elastic Energy and Moiré Patterns: Unraveling the Self-Alignment Mechanism of Pb Nanoislands on Graphene

Oscar Gutiérrez-Varela[a,b*], Roberto Carrasco[c], Iván Brihuega[c], and J.G. Vilhena[a*]

[a]Instituto de Ciencia de Materiales de Madrid, Consejo Superior de Investigaciones Científicas, Madrid, Spain
[b]Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, Madrid, Spain
[c]Departamento de Física de la Materia Condensada, Universidad Autónoma de Madrid, Madrid, Spain

*oscarj.gutierrez@uam.es, guilherme.vilhena@csic.es

Moiré structures in nanocontacts have recently attracted significant attention due to their potential applications in fields such as nanoelectronics and tribology [1,2]. Scanning tunneling microscopy (STM) experiments conducted at cryogenic temperatures on Pb nanoislands deposited on graphene reveal that these islands consistently align along a preferred direction, specifically the zigzag direction of graphene. Moreover, nanomanipulation experiments with STM demonstrate that this alignment is strongly robust, persisting even when the islands move across different graphene domains. To investigate the underlying mechanisms of this alignment, Molecular Dynamics simulations were performed. These simulations reveal that when a nanoisland is initially misaligned (i.e., not in the zigzag direction), it undergoes a spontaneous rotation to achieve the preferred orientation. The calculations also disclose that this rotation is driven by the formation of Moiré patterns in the out-of-plane structure of graphene, with the elastic energy of graphene playing a key role in reorienting the island. These findings have important implications for emerging technologies such as twistronics, where the orientation of nanoclusters on a substrate can significantly influence electronic properties. Understanding and controlling such alignment mechanisms could open new avenues for designing advanced nanoscale devices.

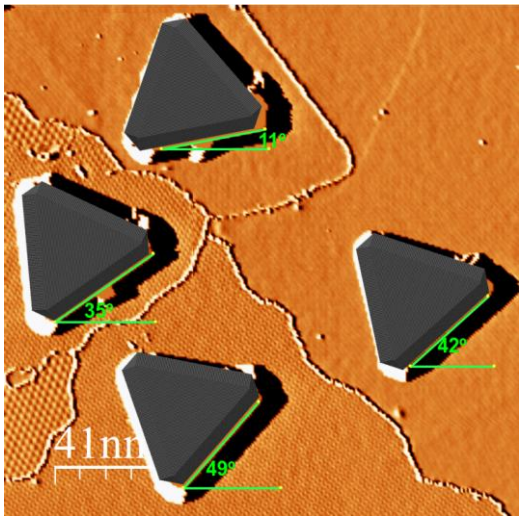

Figure - STM images showing lead nanoislands on graphene consistently aligned with their edges along the zigzag direction of the graphene lattice. For reference, the nanoislands used in MD are overlaid in gray on the images.

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SPM-Based Characterization of Dielectric Layers for Enhanced 2D Device Functionality

J. Hernández-Ruiz [a*], T. Pucher [a], E. Sánchez-Viso [a], V. Zamora [b], V. Rouco [b], J. Santamaria[b], A. Castellanos-Gómez [a], C. Munuera [a]

[a] 2D Foundry research group. Instituto de Ciencia de Materiales de Madrid (ICMM-CSIC), Madrid, Spain.
[b] GFMC, Department Fisica de Materiales, Facultad de Fisica, Universidad Complutense Madrid, Spain.

* julia.hernandez@icmm.csic.es

Two-dimensional (2D) semiconductors, such as MoS2, have gained attention for next-generation devices due to their thin nature and excellent optoelectronic properties [1]. The development of 2D-based devices, including field-effect transistors (FETs), photodetectors and memory devices, relies on the successful integration with high-performance dielectric layers, since they play a key role in performance, power consumption and scalability. To optimize performance, an ideal dielectric should fulfill a number of requirements, including high dielectric constant, low leakage or a wide bandgap.

Although conventional dielectrics like SiO2 are widely used in the semiconductor industry, they are not ideal for 2D-based devices due to its low dielectric constant, high interfacial trap density and charge scattering. Consequently, research into new dielectrics has gained significant focus in recent years, with materials such as hexagonal boron nitride (hBN) [2], valued for its insulating capabilities and smooth surface, and other alternative dielectrics are emerging as focal points of investigation.

These novel dielectrics are often being manipulated in a freestanding form [3], which facilitates the fabrication of 2D-material-based devices but, in some cases, complicates dielectric characterization. As a result, dielectric constant values are often assumed to be similar to those of continuous films. In this work, we present a characterization method using c-AFM that enables direct measurement of the dielectric constant in 2D systems.

Furthermore, if the dielectric material exhibits an additional property, it can enable new mechanisms of control over the device, expanding its functionality beyond conventional operation. Besides the high dielectric constant, BTO offers the possibility to act on its ferroelectric polarization to tune the optoelectronic properties of MoS2-based devices [4]. By combining advanced SPM modes such as KPFM and PFM we have investigated the synergistic interplay between MoS2 and BTO in FET configurations.

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Multireference STS theory of strongly correlated molecules

Manish Kumar [a], Diego Soler [a], **Pavel Jelinek** [a]

[a] Institute of Physics of the Czech Academy of Sciences

* jelinekp@fzu.cz

Recent progress in on-surface synthesis has enabled the preparation of polyradical strongly correlated molecules [1], which are not available by traditional synthetic approaches in solution. However, the characterization of the electronic structure of such molecules with non-trivial electronic structure using scanning tunneling microscopy (STM) provides new challenges. First, interpreting scanning tunneling spectroscopy (STS) maps of the polyradical molecules based on standard one-electron STM theory [2] often fails. Thus, for a precise interpretation of STS maps and their connection to the electronic structure of molecules, a theoretical description, including non-equilibrium tunneling processes going beyond one-electron molecular orbitals, is required. In this talk, we will discuss a many-body theoretical framework that enables us to simulate STS maps accurately [3]. Namely, we will introduce the concept of Dyson orbitals [4] to interpret ionic resonances in STS maps and natural transition orbitals [5] describing spin excitations in STS maps. Finally, we will discuss Kondo orbitals [6] to understand the origin of the spatial Kondo signal in high-spin molecules on metal surfaces.

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On-surface gold-catalyzed hydroamination/cyclization reaction of alkynes

Alejandro Jiménez-Martín [a,b], Tatiana Munteanu [c], Qifan Chen [b], Simon Pascal [c], Aura Tintaru [c], Benjamin Mallada [a], Pingo Mutombo [b], Olivier Siri [c], Pavel Jelínek [b] and Bruno de la Torre [a]

[a] Regional Centre of Advanced Technologies and Materials, Czech Advanced Technology and Research Institute (CATRIN) Palacký University, 78371 Olomouc, Czech Republic
[b] Institute of Physics of the Czech Academy of Science, 16200 Prague, Czech Republic
[c] Aix Marseille Univ., CNRS UMR 7325 Centre Interdisciplinaire de Nanoscience de Marseille (CINaM), 13288 Marseille, France

* alejandro.jimenezmartin@upol.cz

On-surface synthesis under ultra-high vacuum (UHV) conditions facilitates the fabrication of unique molecular compounds, replicating established in-solution protocols. However, the intramolecular hydroamination and cyclization (IHC) of alkynes on surfaces remain unexplored due to the challenges posed by the repulsion between the nitrogen lone pair and the alkyne π-system. Here we describe the first on-surface IHC of alkyne-functionalized molecular precursors in UHV environment on the Au(111) surface.

Notably, the synthesis introduces two pyrrole groups into the quinoidal-based precursor, enabling the formation of two fused pyrrolo-benzoquinonediimine compounds not achievable in solution chemistry. To analyze the resulting reaction products, we utilized scanning tunneling microscopy and non-contact atomic force microscopy with single bond resolution, comparing these products to those obtained through solution methods. In parallel to the experimental results, we provide a detailed computational description of the key role of a single gold adatoms during the complete on-surface reaction.

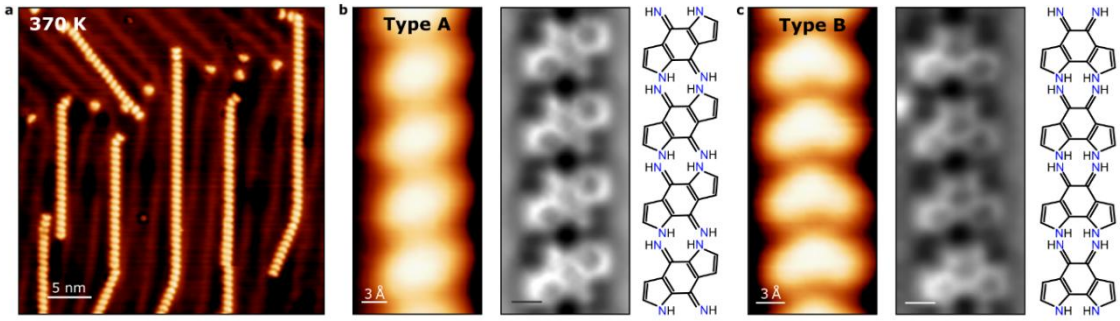

Figure 1. On-surface characterization of N-heterocyclic compounds. a) STM topographic overview image after annealing the sample at 370K. STM, nc-AFM and chemical model of b) Type A and c) Type B chains.

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In-situ AFM and GIWAXS for the real-time monitoring of MOF degradation in controlled humidity environments

M. Linares-Moreau [a*], L. A. Brandner [a], H. Amenitsch [b], P. Falcaro [a]

[a] Institute of Physical and Theoretical Chemistry, Graz University of Technology, 8010 Graz, Austria

[b] Institute of Inorganic Chemistry, Graz University of Technology, 8010 Graz, Austria

* mlinaresmoreau@icmab.es

*Present affiliation: Institut de Ciència de Materials de Barcelona (ICMAB), CSIC, Campus Bellaterra, 08193 Barcelona, Spain

3D-oriented metal-organic framework (MOF) films and patterns have recently emerged as promising platforms for sensing and photonic applications [1]. These oriented polycrystalline materials are typically prepared by heteroepitaxial growth from aligned inorganic nanostructures and display anisotropic functional properties, such as guest molecule alignment and polarized fluorescence [2]. However, a crucial aspect for the integration of these materials into functional devices is the evaluation of their environmental stability, in particular, towards water and high humidity. In this work, we present an in-depth analysis of the structural evolution of aligned 2D and 3D Cu-based MOFs grown from $Cu(OH)_2$ substrates [3]. Specifically, 3D-oriented Cu_2L_2 and Cu_2L_2DABCO films (L = 1,4-Benzenedicarboxylate, BDC; Biphenyl-4,4-dicarboxylate, BPDC; DABCO = 1,4-Diazabicyclo[2.2.2]octane) were exposed to 50% relative humidity (RH), 80% RH and liquid water. The combined use of X-ray diffraction, infrared spectroscopy, atomic force microscopy (AFM) and electron microscopy shows that the sensitivity towards humid environments critically depends on the presence of the DABCO pillar ligand. While oriented films of 2D MOF layers stay intact upon exposure to all levels of humidity, hydrolysis of Cu_2L_2DABCO is observed. In addition, we report that in environments with high water content, 3D-oriented $Cu_2(BDC)_2$DABCO recrystallizes as 3D-oriented $Cu_2(BDC)_2$. This heteroepitaxial MOF-to-MOF transformation mechanism was studied with in-situ synchrotron experiments and time-resolved AFM measurements in controlled humidity environments. In this presentation, we highlight how environmental time-resolved AFM and grazing incidence wide-angle X-ray scattering (GIWAXS) measurements can be used as complementary methods to monitor the changes in crystallinity, particle size and morphology during a MOF degradation/transformation process. These findings provide valuable information on the stability of oriented MOF films for their application in functional devices and highlight the potential for the fabrication of 3D-oriented superstructures via MOF-to-MOF transformation.

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Electronic structure tunability ofcarbon-based 1D-polymers combining cross-conjugation and nitrogen doping

Adriana E. Candia [a,b,c], M. Vilas-Varela [d], M. H. Aguirre [e,f], C. Rogero [b], D. Serrate [a,e,f], D. Peña [d], **J. Lobo-Checa** [e,f].

[a] Laboratorio de Microscopias Avanzadas (LMA), Universidad de Zaragoza, Spain.
[b] Centro de Física de Materiales (CSIC-UPV/EHU), San Sebastián, Spain.
[c] Instituto de Física del Litoral, Consejo Nacional de Investigaciones Científicas y Técnicas, Universidad Nacional del Litoral, Santa Fe, Argentina.
[d] Centro Singular de Investigación en Química Biolóxica e Materiais Moleculares (CiQUS) and Departamento de Química Orgánica, Universidade de Santiago de Compostela, Spain.
[e] Departamento de Física de la Materia Condensada, Universidad de Zaragoza, Spain.
[f] Instituto de Nanociencia y Materiales de Aragón (INMA), CSIC-Universidad de Zaragoza, Spain.

* jorge.lobo@csic.es

Quasi-one-dimensional polymer structures with extended π-electron systems stand out due to their remarkable application in light-emitting diodes and devices. Upon smart choice of their building units, such carbon-based organic nanoarchitectures provide excellent optoelectronic properties by tuning their dimensionality, atomic structure or intrinsic doping. Here, we generate and study three canonical cross-conjugated quasi one-dimensional chains with controlled nitrogen intrinsic doping, which is selectively introduced into their poly-phenylene backbones (see Figure). By means of scanning tunneling microscopy and spectroscopy we corroborate that the cross-conjugation that break the chain linearity is exclusively responsible of the electronic confinement in the straight segments [1]. Moreover, we demonstrate that the LUMO state exhibits the same spatial distribution for the cross-conjugated polymers independently of the pyridine content of the initial precursor (see Figure). Despite this coincidence, the semiconducting character and other relevant electronic properties of the polymers are found to depend on both the chain morphology and the precise position and number of doping nitrogen atoms synthetically introduced into the molecular precursors. We compare these results to related previous studies [1-3], which allows us to unambiguously validate the opto-electronic tunability upon the choice of the polymers' building units [4].

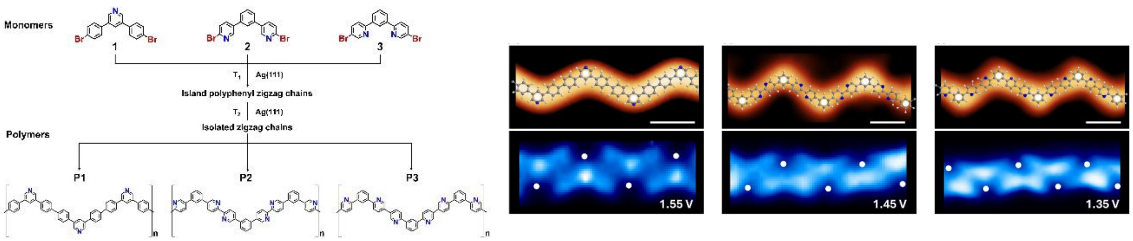

Figure – Schematic representation of the precursor molecules and on-surface synthesized polymeric chains. The spatial distribution of the LUMO state coincides for the three cross-conjugated chains, but the observed energy shift is dependent on the precise position and number of doping nitrogen atoms embedded in the structure.

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Cryogenic, ultrahigh vacuum sample transfer between electrospray ion beam deposition (ESIBD) and scanning probe microscopy (SPM)

A. Lynch Gonzalez [a], L. Eriksson [a], M. Grabarics [a], T. Esser [a], B. Mallada [a], S. Rauschenbach [a]

[a] University of Oxford

alejandro.lynchgonzalez@chem.ox.ac.uk

Electrospray ion beam deposition (ES-IBD) is currently the only viable method for cleanly and selectively depositing large and complex molecules which do not have a vapour pressure while preserving their chemical structure. In our lab, ESIBD[1] and SPM instruments are physically separate and sample transfer between them is performed using a vacuum suitcase system which maintains UHV and cryogenic conditions during transfer, essential for suppressing surface diffusion, conformational changes, and contamination during the transfer. Here, we present the design, implementation, and benchmarking of a cryogenic UHV suitcase and showcase applications.

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Electrospray Deposition of Porphyrin Nanorings on Graphene/Ir(111) Surface

Himani Malik [a], Alejandro Jiménez-Martín [a], Benjamin Mallada [a,b], Harry L. Anderson [c], Pavel Jelinek [a,d], and Bruno de la Torre [a,e]

[a] Regional Centre of Advanced Technologies and Materials, Czech Advanced Technology and Research Institute (CATRIN), Palacký University, 78371 Olomouc, Czech Republic.
[b] Kavli Institute for Nanoscience Discovery, University of Oxford, OX1 3TA, UK
[c] Chemistry Research Laboratory, University of Oxford, OX1 3TA, UK
[d] Nanosurf Lab, Institute of physics of the Czech Academy of Science, 16200 Prague, Czech Republic
[e] Nanomaterials and Nanotechnology Research Center (CINN), CSIC-UNIOVI-PA, 33940 El Entrego, Spain

* himani.malik@upol.cz

Porphyrin complexes are promising building blocks for optical devices, sensors, and electronics due to their extended conjugation, tunable chromophore interactions, and strong UV–Vis absorption. As the central component of chlorophyll, porphyrins enable solar-to-chemical energy conversion. Synthetic porphyrin nanostructures—such as rings, tubes, and ribbons—emulate natural light-harvesting systems, offering controllable electronic properties, efficient charge transport, and long exciton lifetimes. Ring-shaped porphyrin complexes support aromatic or antiaromatic ring currents depending on their redox state. These currents enable coherent charge and exciton delocalization across the nanoring, with tunable inter-unit communication. However, probing these processes is limited by current experimental resolution, ensemble averaging, and spectral assignment challenges, often requiring simulations that depend on adjustable parameters and offer limited predictive power.

Here, we directly image the real-space electronic structure of a single porphyrin nanoring consisting of twelve porphyrin units connected by butadiyne spacers. Due to their incompatibility with vacuum sublimation, we use electrospray deposition from a (3:1) toluene:methanol mixture. Solubility is enhanced by OC8H17 alkyl side chains on the porphyrin cores. The nanorings are deposited on monolayer graphene on Ir(111) to preserve their intrinsic electronic features. Scanning probe microscopy reveals their structure, conformation, and surface interactions at the atomic scale. Tunneling spectroscopy combined with sub-molecularly resolved conductance maps, uncovers the complex intra-ring electronic landscape of these macrocycles, enabling the analysis of electron distribution—both coherent and incoherent—within the ring.

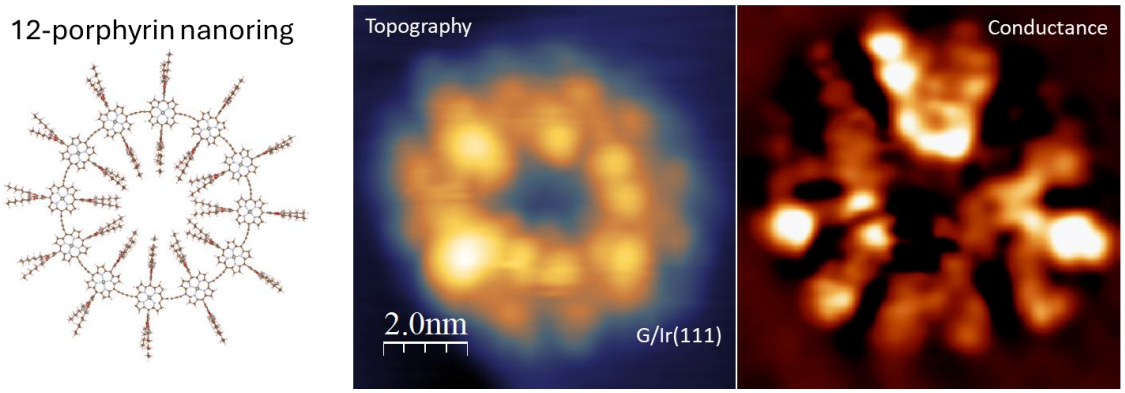

Fig1. (left) c-P12 molecular structure, (center) STM topograph of c-P12 molecule deposited on graphene/Ir(111) surface by electrospray. (right) Sub-molecularly resolved conductance map of a single porphyrin nanoring.

Atomic-Scale Sequencing of Sulphated Glycans

B. Mallada* [a,b,c], M. Grabarics [a,b], W. B. Struwe[a,b], R. L. Miller[d], B. de la Torre[e], S. Rauschenbach[a,b,c]

[a] Kavli Institute for Nanoscience Discovery, University of Oxford, Oxford, UK
[b] Department of Biochemistry, University of Oxford, Oxford, UK
[c] Department of Chemistry, University of Oxford, OX1 3QU, Oxford, UK
[d]Copenhagen Center for Glycomics, Department of Cellular and Molecular Medicine, University of Copenhagen, Copenhagen, DK-2200, Denmark
[e] Nanomaterials and Nanotechnology Research Center (CINN) CSIC-UNIOVI-PA, 33940 El Entrego, Spain

* benjamin.mallada@bioch.ox.ac.uk

Sulphated glycans, particularly Glycosaminoglycans (GAGs), are essential biomolecules that regulate a range of critical biological functions, including cell signaling, tissue repair, and immune response. Their highly sulfated nature enables them to interact with growth factors, cytokines, and receptors, influencing processes such as wound healing, cell migration, and inflammation.

Using low temperature STM, KPFM, and nc-AFM, we have successfully sequenced complex sulphated glycans, overcoming the limitations of conventional methods such as mass spectrometry and NMR, which struggle with branched or heterogeneous structures. While STM [1] provides high-resolution imaging of surface structures, nc-AFM offers deeper insights by probing atomic-level interactions, such as electrostatic forces and non-covalent interaction, which STM cannot capture accurately. This allows us to precisely identify single functional groups on glycan surfaces, unlocking new possibilities for understanding their roles in cellular processes and advancing applications in diagnostics, therapeutics, and precision medicine.

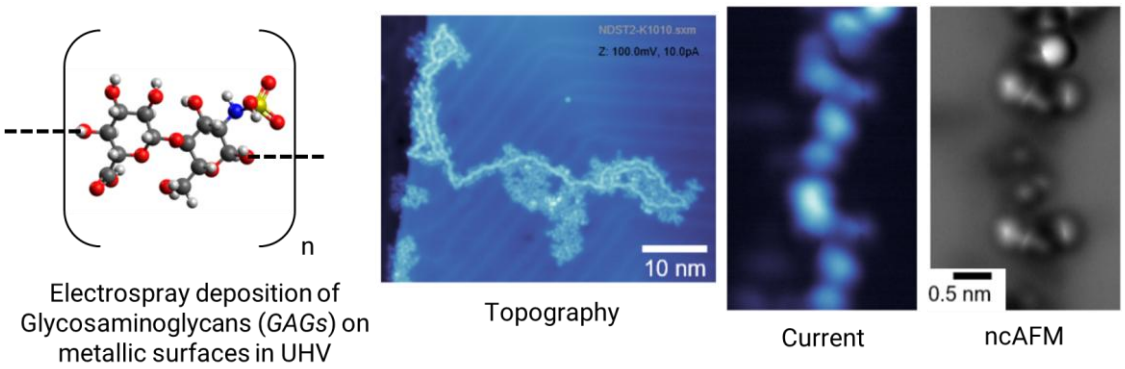

Figure – Glycosaminoglycan model deposited on Au(111) with topographic and constant height measurements.

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On-Surface Synthesis of Porphyrinoid-Based Derivatives Comprising Exotic Macrocycles.

Alberto Martínez[a]*, Maxence Urbani[a,b],Ana Barragán[a], Koen Lauwaet[a], Jose María Gallego[a], Aurelio Gallardo[a], Rodolfo Miranda[a], David Écija[a], Tomás Torres[a,b], José Ignacio Urgel[a]

[a] IMDEA Nanociencia, C/ Faraday 9, Campus de Cantoblanco, 28049 Madrid, Spain [b] Departamento de Química Orgánica and Institute for Advanced Research in Chemistry (IAdChem), Universidad Autónoma de Madrid, 28049 Madrid, Spain

* alberto.martinez@imdea.org

The synthesis of porphyrinoid-based compounds has attracted the interest of many surface scientists during the last decades due to their intriguing electronic, optical and catalytic properties. In this work, porphyrinoid-based derivatives with exotic macrocycles (6 & 7 nitrogen hemiporphyrazines) have been fabricated on Au(111) and studied with the use of Scanning Tunneling Microscopy (STM) and non-contact Atomic Force Microscopy (nc-AFM) under ultrahigh-vacuum conditions (UHV), complemented by theoretical modeling. Particularly, through surface-assisted synthesis, three carbahemiporphyrazines of distinct dimensionality equipped with isopropyl groups have been studied. As shown in *Figure 1*, the macrocycle of precursors **P1** and **P2** comprises two pyrrole units and two benzene rings, while in precursor **P3** one of the benzene rings has been substituted by a pyridine.

First, an intermolecular carbon-carbon coupling between the carbahemiporphyrazine precursors was achieved by thermal activation of their isopropyl substituents via a [3+3] cycloaromatization, giving rise to dimers (0D), one- and two dimensional (1D and 2D) polymers. Second, the three low-dimensional free-base macromolecules, were exposed to an atomic flux of cobalt atoms, giving rise to cobalt-metalated macrocycles. The dicarbahemiporphyrazines **1** and **2** showed that the metal atoms were coordinated only to the two pyrrolic nitrogens, in contrast to the typical four-fold coordination that occurs inside tetrapyrroles, while the monocarbahemiporphyrazine **3** shows a three-fold coordination. This on-surface protocol renders atomically precise covalently-linked carbahemiporphyrazine-based derivatives, and provides promising model systems toward the exploration of metallated, low-coordinated, porphyrinoid systems with utility in diverse technological areas.

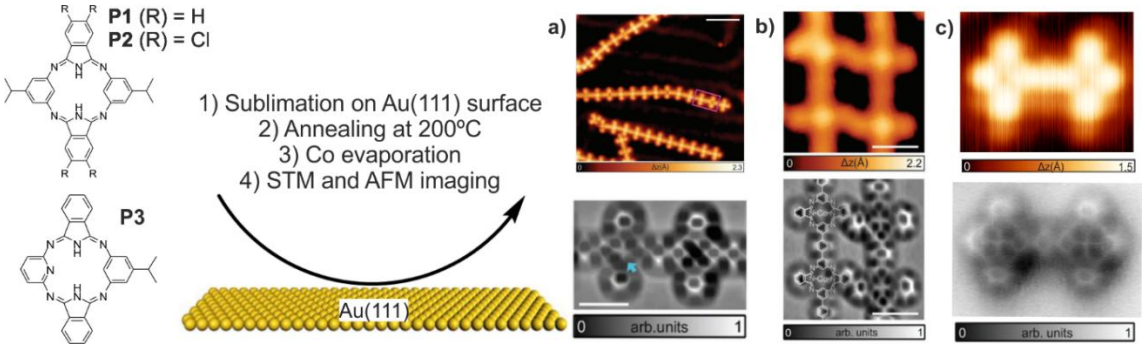

Figure 1. Scheme of work and characterization of: a)-b) STM and Laplace-filtered constant-height frequency shift nc-AFM images of evolved **P1 & P2**. c) STM and constant-height frequency shift nc-AFM images of evolved **P1.**

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Cyclodehydrogenation of nanographene molecular precursors catalyzed by atomic hydrogen

Rafal Zuzak [a], Pawel Dabczynski [a], Jesús Castro [b], **José I. Martínez** [c,*], Mads Engelund [d], Dolores Pérez [b], Diego Peña [b], Szymon Godlewski [a]

[a] Faculty of Physics, Astronomy and Applied Computer Science, Jagiellonian University
[b] CiQUS and Departamento de Química Orgánica, Universidade de Santiago de Compostela
[c] Instituto de Ciencia de Materiales de Madrid (ICMM-CSIC)
[d] Espeem S.A.R.L. (espeem.com)

* joseignacio.martinez@icmm.csic.es

The present work [1] is aimed toward controlling the atomically precise on-surface synthesis of graphene-based nanostructures regardless of the type of substrate used, a grand scientific challenge that cuts across physics, chemistry, materials science and nanoelectronics. A barrier that has to be surmounted to achieve this goal is the need to overcome the limitations resulting from the hitherto irreplaceable catalytic role of the substrate in the on-surface synthesis of graphene derivatives. In this investigation we present the first experimentally achieved protocol, which allows to perform an on-surface reaction independently from the substrate. We demonstrate a completely new reaction pathway, which is based on replacing the catalytic role of the substrate by an externally dosed gaseous catalyst - an approach that to the best of our knowledge has not yet been proposed in the surface assisted synthesis. The new synthetic approach benefits from the completely counterintuitive application of atomic hydrogen to catalyze the cyclodehydrogenation reaction for planarizing the molecular precursors, which yield the graphene-based nanostructures. Basing the protocol on the externally dosed hydrogen as catalyst, ensures independence from the type of applied surface. Using this approach, we have manufactured differently shaped graphene moieties on a range of surfaces starting from metallic (Au), through semiconducting (TiO_2 and Ge:H), to insulating (Si/SiO_2 and NaCl layers) demonstrating the vast versatility and broad scope of our method. The use of such a wide range of materials required also overcoming barriers in obtaining precise identification of the chemical reaction products. This was achieved through the involvement of complementary techniques such as scanning tunneling microscopy and spectroscopy (STM/STS), non-contact atomic force microscopy (nc-AFM) and secondary ion mass spectrometry (SIMS), corroborated by state-of-the-art first-principles theoretical simulations, which provided the atomic-scale insight into the mechanism of the hydrogen-catalyzed cyclization. The consequences of our findings are far-reaching. We have discovered and utilized a completely new reaction pathway yielding graphene nanostructures on a range of surfaces, including those technologically most interesting and demanded. These findings are highly relevant for chemists and material scientists delivering synthetic routes toward new functional materials, especially merging low-dimensional functional devices with atomically precise and monodisperse graphene units.

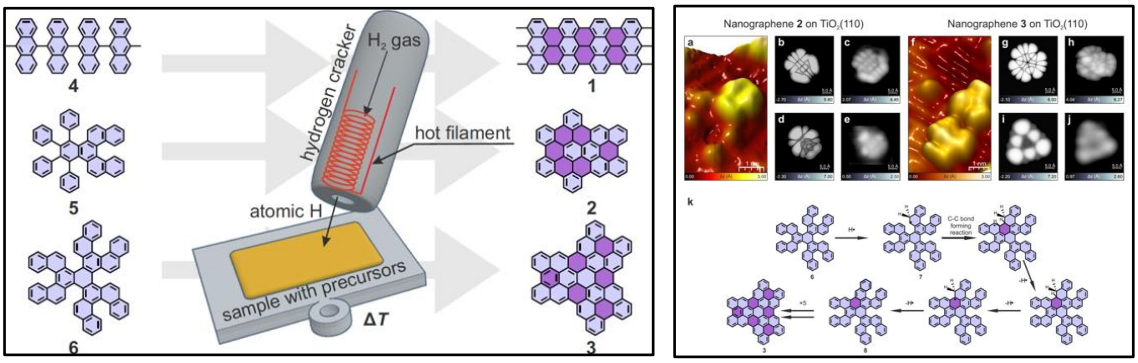

Figure - (Left panel) Cyclodehydrogenation catalyzed by atomic hydrogen scheme, and (right panel) Atomic hydrogen induced planarization yielding nanographenes 2 and 3 on TiO_2(110)-(1×1)

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Upgrade of a variable temperature scanning tunneling microscope for nanometer-scale spectromicroscopy

B. Cirera [a], A. Sáez-Coronado [a], D. Arribas [a], J. Méndez [a], A. Sagwal [b c], R. de Campos Ferreira [b], M. Švec [b d], **P. Merino [a]**.

[a] Material Science Institute of Madrid (ICMM-CSIC), 28049, Spain.
[b] Institute of Physics, Czech Academy of Sciences; Praha, Czech Republic.
[c] Faculty of Mathematics and Physics, Charles University; Praha, Czech Republic.
[d] Institute of Organic Chemistry and Biochemistry, Czech Academy of Sciences; Flemingovo náměstí 542/2, Praha 6 CZ160 00, Czech Republic.

* pablo.merino@csic.es

Tip-enhanced Raman spectroscopy (TERS), tip-enhanced photoluminescence (TEPL), and scanning tunneling microscope-induced luminescence (STML) combine the high spatial resolution of probe microscopies with the spectroscopic capabilities of optical techniques. Here, we describe the upgrade of an ultrahigh vacuum (UHV) variable-temperature scanning probe microscope (VT-SPM) to perform tip-enhanced spectromicroscopy experiments at cryogenic temperatures. The home-made design includes a portable focusing lens (NA=0.45) that allows the simultaneous collection and injection of light from the tip-sample junction while assuring easy tip and sample transfers. We demonstrate the capabilities of our upgrade to resolve electroluminescence (EL), Raman, and TERS spectra using plasmonically active probes (Ag and Au tips) on various surfaces. We are able to observe the vibrational levels of C_{60} deposited on Ag(111) with a lateral resolution of ~2 nanometers. Moreover, we use the tunability of the gap plasmon distribution to observe intense anti-Stokes signals of C_{60}, highlighting the spectral sensitivity of the system. This upgrade opens new possibilities for studying surface chemistry, catalysis, and molecular electronics at state-of-the-art spatial and spectral resolutions using accessible VT-SPM systems. The 3D CAD files and detailed step-by-step methodology is provided in Ref. [1] in an open-science effort to expand light-matter interaction experiments in the SPM community.

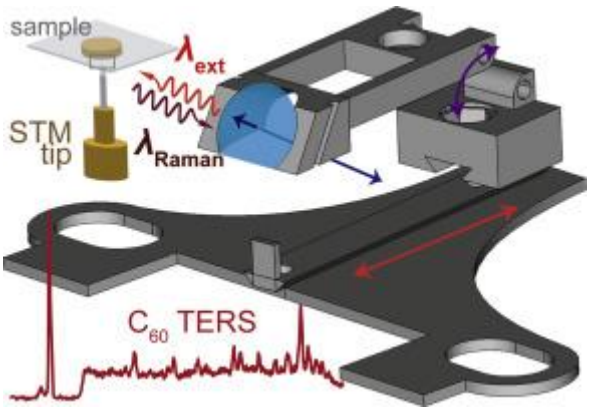

Figure - View of the STEP file of our custom-designed mobile lens support, highlighting its three different structures: the anchoring platformt to the SPM platform, the angle-tuning mechanism and the wobble-stick pushed-up slider (red arrow). Sample and tip are also represented and the inset introduces a UHV-TERS spectrum of a C_{60} layer on Au(111).

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Two-tone measurements on a single nuclear spin using ESR-STM

H. G. Vennema [a], **C. Mier González** [a], E. W. Stolte [a], J. Lee [a], L. Edens [b] , S. Otte [a]

[a] Delft University of Technology, Delft, The Netherlands
[b] CIC-nanoGUNE, Donostia-San Sebastian, Spain

* c.miergonzalez@tudelft.nl

Nuclear spins exhibit a high degree of isolation from their environment, resulting in long lifetimes and coherence times. This makes nuclear spins a promising platform for the development of quantum technologies [1]. The combination of Electron Spin Resonance (ESR) with STM has enabled the indirect measurement of nuclear spins on single atoms via the hyperfine interaction [2]. More recently, single-shot readout on Ti isotopes has demonstrated a nuclear lifetime of about 5 seconds [3]. In this work we aim to controllably address nuclear spin transitions using ESR-STM. Specifically, we propose a two-tone measurement scheme to drive and readout the nuclear spin resonances (NMR) on a ^{47}Ti isotope (I = 5/2). Our study paves the way for the coherent manipulation of single nuclear spins using STM.

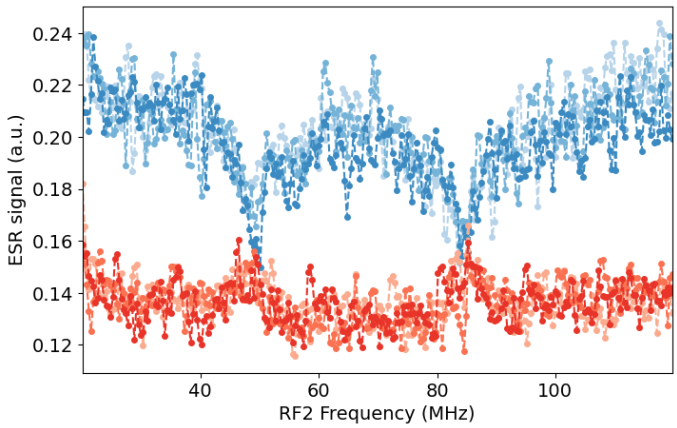

Figure – Two-tone NMR spectroscopy on a single ^{47}Ti isotope.

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Epitaxial growth of superconducting proximitized Au films on Nb

Katerina Vaxevani [a], **Georg Monninger** [a], Dongfei Wang [a,b], Stefano Trivini [a], Johannes Wolf [a], Jon Ortuzar [a], Jose Ignacio Pascual [a,c]

[a] CIC nanoGUNE-BRTA, 20018 Donostia-San Sebastián, Spain
[b] School of Physics, Beijing Institute of Technology, Beijing 100081, China
[c] Ikerbasque, Basque Foundation for Science, 48013 Bilbao, Spain

* g.monninger@nanogune.eu

Novel applications in quantum technology require new classes of superconducting materials. As a candidate for quantum computing and data storage, the spin excitation times of magnetic molecules can be enhanced by placing them on a superconductor [1]. We study the epitaxial growth of gold thin films on superconducting Nb(110) with low-temperature scanning tunneling microscopy (STM) and investigate the dependence of the surface state energy and the character of the surface reconstruction on coverage and annealing conditions. We find that the surface morphology remains intact upon post-annealing (Fig. 1). We confirm the opening of a superconducting gap of the proximitized gold substrate through scanning tunneling spectroscopy (STS). Our work shows a promising platform for on-surface synthesis of magnetic molecules for probing their interaction on a proximitized superconductor.

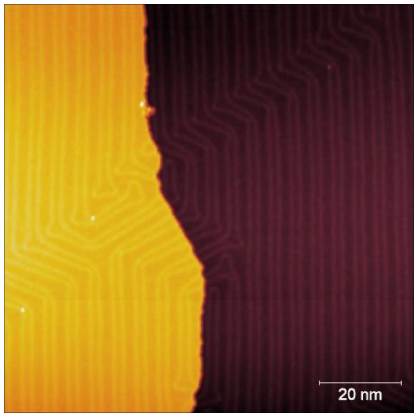

Figure – STM image of proximitized Au

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Spin-split edge states in metal-supported graphene nanoislands

M. Gastaldo[a], M. Massoud[b], C. Garcia Fernandez[c], D. Sánchez-Portal[c], A. Garcia-Lekue[d,e], G. Ceballos[a], and **A. Mugarza[a,f,*]**

[a]Catalan Institute of Nanoscience and Nanotechnology (ICN2), CSIC and BIST, Bellaterra, 08193 Barcelona, Spain
[b]Universidad Autónoma de Madrid, Madrid, E-28049 Spain
[c]Centro de Física de Materiales (CFM) CSIC-UPV/EHU, E-20018 Donostia-San Sebastián, Spain
[d]Donostia International Physics Center, Paseo M. de Lardizabal 4, 20018 San Sebastian, Spain
[e]Ikerbasque, Basque Foundation for Science, Bilbao, Spain
[f]ICREA—Institució Catalana de Recerca i Estudis Avançats, 08010 Barcelona, Spain.

* aitor.mugarza@icn2.cat

Spin-split states localized on zigzag edges have been predicted for different freestanding graphene nanostructures [1]. However, the stability of the edge magnetism can be severely influenced by interfacial interactions when supported on metallic substrates [2]. This imposes a serious challenge for the on-surface synthesis of magnetic graphene nanostructures. In this work we demonstrate that on-surface synthesized graphene nanoislands with well-defined zigzag edges can retrieve their spin-split edge states by minimizing interfacial interactions through metal intercalation [3]. Using scanning tunneling microscopy and spectroscopy we detect edge states with subnanometer spatial localization and 1.2 eV energy splitting, comparable to the spin-polarized states predicted by ab-initio calculations.

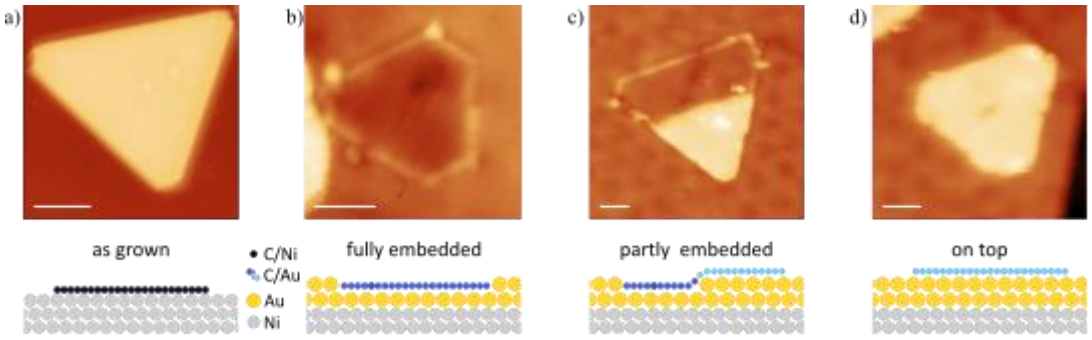

Figure 1 - Graphene nanoislands (GNI) on intercalated Au films. Representative STM images and corresponding schematics of GNI configurations (a) on Ni(111) and (b-d) after Au intercalation.

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On Surface synthesis of a 2D carbon nitride metal-coordinated network

J. M. Zamalloa-Serrano[a], J. I. Mendieta-Moreno[a], J. M. Gómez-Fernández[a], M. F. López[a], C. Sánchez-Sánchez[a], J. I. Martínez[a], J. A. Martín-Gago[a] and **I. Palacio[a]**

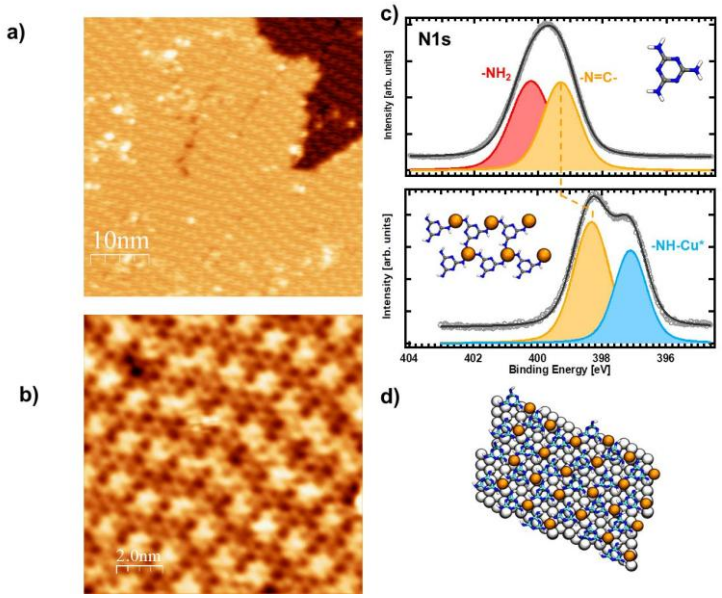
[a] Institute of Material Science of Madrid (ICMM-CSIC), C/Sor Juana Inés de la Cruz 3, 28049 Madrid, Spain

* i.palacio@csic.es

2D metal-coordinated networks combine the heterogeneous catalytic properties of organic ligands with a defined coordination geometry, identifiable active centers and on-demand ligand moieties resulting in enhance efficiency and specificity in the catalytic reaction making them ideal SAC with a broad range of applications in the green hydrogen production or the treatment of environmental pollutants. They can be synthesized by on-surface synthesis, a bottom-up strategy offering atomic-level control and utilizing the intrinsic surface adatoms of reactive metallic substrates.

In this work, we have investigated the formation of a 2D metal-coordinated carbon nitride network synthesized by taking advantage of the heterogeneous single-metal-site catalysts of an adatom-filled Cu(110) surface and using melamine molecules as an organic precursor. At a temperature of 600 K, melamine molecules undergo partial dehydrogenation of the amino groups, followed by subsequent metalation with the native copper adatoms. This process results in the formation of a hexagonal 2D Cu-coordinated carbon nitride network, distinguished by a Cu(I) oxidation state. The generated 2D network has been characterized by means of scanning tunnelling microscopy (STM), X-Ray photoelectron spectroscopy (XPS) and QM/MM. These investigations lead to main conclusions underscoring the pivotal role of copper adatoms, acting as atomic catalysts in the dehydrogenation process and stabilizers of the resulting network.[1]

Figure - a) STM image (I = 0.05 nA; V = 1 V) of the obtained metal-coordinated network on a Cu(110)



substrate. b) Zoom of a). c) N1s core level of a melamine multilayer and the metal-coordinated network, respectively. The inset of c) shows a schematic representation of a melamine molecule and of a scheme of the network. d) Top view of a 2x2 unit cell after a MD simulation at 300 K.

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Competition between Coulomb blockade and superconducting correlations in Pb islands on graphene

Jon Ortuzar [a], Stefano Trivini [a], Katerina Vaxevani [a], Beatriz Viña Bausà [a,b], Sebastian Bergeret [c], **Nacho Pascual [a]***

[a] CIC nanoGUNE, San Sebastián – Donostia, Spain
[b] Universidad Autónoma de Madrid, Madrid, Spain
[c] Centro de Física de Materiales (CFM),San Sebastián - Donostia, Spain

* ji.pascual@nanogune.eu

Non-reciprocity is a fundamental principle in electronics, essential for current rectification. It implies that electrical conductance depends on the current direction, enabling key functionalities such as transistor operation, signal detection, and light emission. In superconducting electronics, developing non-reciprocal effects to control supercurrents and Cooper pair flows is a pressing challenge. Although several mechanisms have been proposed and observed, achieving non-reciprocal superconducting currents without external magnetic fields remains difficult.

Here, we demonstrate that small lead islands grown on graphene exhibit non-reciprocal effects driven by the interplay between superconducting pairing — attractive at low temperatures — and Coulomb blockade — repulsive in nature. We find that these islands display a larger and asymmetric superconducting gap compared to bulk superconductors. This asymmetry arises from quasiparticle excitations at the gap edge, modified by Coulomb blockade, as explained using a double tunneling junction model.

In the Josephson regime, we observe the splitting of Josephson peaks into Resonant Cooper Pair Tunneling (RCT) peaks in the current-voltage characteristics. The RCT energy values shift with gating, which we control via STM tip pulses. Using a current-biased STM junction, we detect Cooper pair tunneling currents that are asymmetric with respect to bias polarity — a clear manifestation of nonreciprocal transport, tunable by an electric gate.

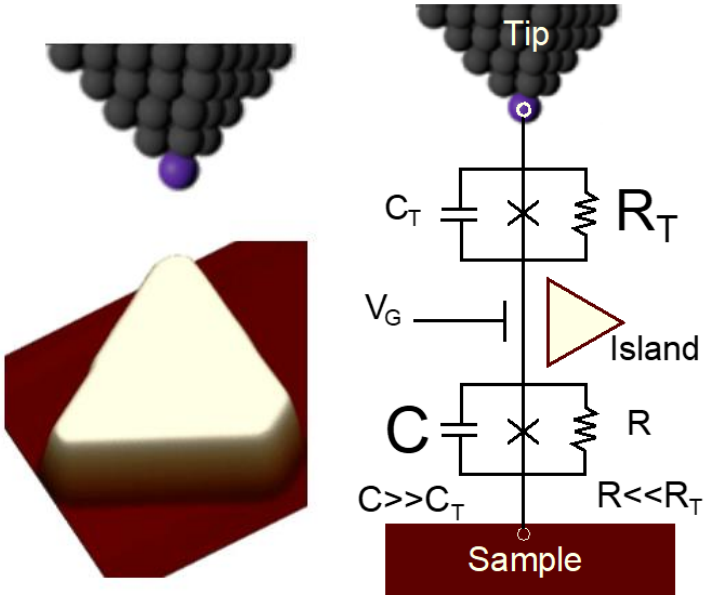

Figure – Three dimensional rendering of a Pb island on graphene, and schematics of the circuit that explains the non-reciprocal transport.

Towards new hybrid graphene nanoarchitectures for gas sensing applications

Esteve Ribas [a], Sara Fiori [a], Luis Mateo [b], Adrián Martínez [b], Diego Peña [b,c], Daniel Herrera [d], Núria Aliaga-Alcalde [d,e], Aitor Mugarza [a,e]

[a] Catalan Institute of Nanoscience and Nanotechnology (ICN2), CSIC and BIST, Campus UAB, Bellaterra, 08193 Barcelona, Spain
[b] Center for Research in Biological Chemistry and Molecular Materials (CiQUS) and Department of Organic Chemistry, University of Santiago de Compostela, 15782 Santiago de Compostela, Spain.
[c] Oportunius, Galician Innovation Agency (GAIN), 15702 Santiago de Compostela, Spain
[d] Institute of Materials Science of Barcelona (ICMAB-CSIC), Campus UAB, Bellaterra, 08193 Barcelona, Spain
[e] ICREA–Institució Catalana de Recerca i Estudis Avançats, 08010 Barcelona, Spain.

* esteve.ribas@icn2.cat

2D materials appear as the most promising candidates for sensing applications due to their high surface area to volume ratio, where the single atom thickness exposes all atoms to the analyte and the large lateral size maximizes the sensing area, promising maximum miniaturization and sensitivity. The robustness and flexibility of 2D materials are also perfectly suited for the design of portable and wearable sensors. Among 2D materials, graphene (Gr) is particularly promising by virtue of its outstanding properties (extremely low resistivity and electronic noise, non-covalent interactions with gases), although its semimetallic character drastically affects its sensitivity and significantly limits its implementation in real devices. An additional drawback of Gr is the lack of selectivity, one of the most important figures of merit of sensors [1]. However, Gr functionalization via reactive sites (e.g. vacancies and pores) is one of the most efficient ways of introducing selectivity and sensitivity to this otherwise rather inert material [2].

Based on results recently published by our group about the growth of semiconducting graphene nanoribbons (GNR) channels with functionalized units [3,4], our aim is to scale in complexity by intercalating non-graphenoid components and GNR, combining semiconducting channels with sensing functional sites. Here we present the advances in the realization of such hybrid Gr nanoarchitectures (HGNs). Our work is focused on nitrogen-containing precursors, as having such heteroatoms in the final structures is interesting for metal coordination, catalysis and sensing applications.

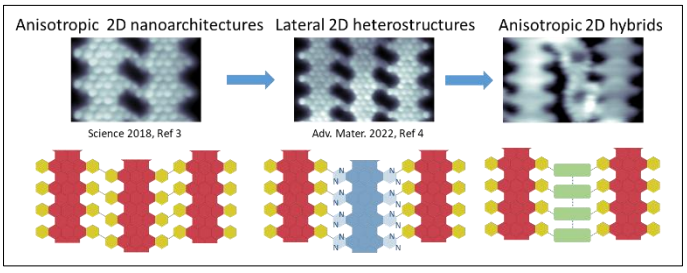

Figure 1 - Outline of the pioneering work done and the ongoing research on 2D hybrids

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Preparation of free-standing twisted bilayer graphene for mechanical properties measurements

P. Romero Proaño [a,b], G. López-Polín [a], J. Gómez-Herrero [b,c]

[a] Departamento de Física de Materiales, Universidad Autónoma de Madrid, Madrid, 28049 Spain
[b] Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, Madrid, 28049 Spain
[c] Departamento de Física de la Materia Condensada, Universidad Autónoma de Madrid, Madrid, 28049 Spain

* pabloandres.romero@uam.es

Stacked two-dimensional (2D) materials with variable twist angles exhibit a diverse range of physical properties, making them valuable for both fundamental research and technological applications. Among them, twisted bilayer graphene (TBG) has gained significant interest due to its unique electronic phases near the magic angle ($\theta \sim 1.1°$). [1] While most studies have focused on its electronic and optical behavior, its mechanical properties remain largely unexplored. Theoretical models predict that below a critical twist angle, moiré-induced structural instabilities may lead to buckling and other out-of-plane deformations in freestanding TBG, potentially impacting its mechanical stability. [2] Here, we introduce a transfer methodology to fabricate freestanding TBG on Si/SiO_2 substrates with predefined circular wells, enabling direct mechanical characterization. The process involves assembling the twisted bilayer on a Si/PVA substrate, transferring it onto a polydimethylsiloxane (PDMS) film, and subsequently transferring it to the Si/SiO_2 substrates with holes. Unlike conventional tear-and-stack techniques, which leave TBG attached to or encapsulated in hexagonal boron nitride (hBN), [3] this approach allows for suspended structures suitable for mechanical measurements such as Young's modulus and thermal expansion coefficient (TEC) through AFM nanoindentation. This experimental configuration provides new insights into the mechanical behavior of twisted 2D systems, paving the way for their integration into mechanically tunable devices.

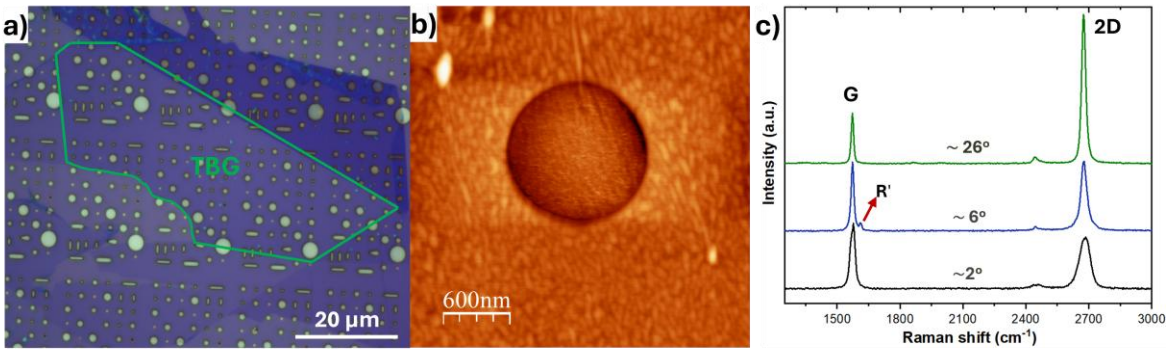

Figure 1 – a) Optical image of a TBG sample on a Si/SiO_2 patterned substrate, b) AFM topography image of a representative TBG drumhead used for nanoindentation measurements, and c) Raman spectra of TBG samples with different twist angles.

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Development of a combined transfer-AFM-transport system to prepare and characterize twisted 2D devices for UHV environments.

L. Romero-Sánchez [a], D. Expósito [a], D. Gallego-Fuente [a], P. Ares [a, b, c], J. Gómez-Herrero [a, b, c], H. González-Herrero [a, b, c], I. Brihuega [a, b, c]

[a] Departamento de Física de la Materia Condensada, Universidad Autónoma de Madrid, E-28049 Madrid, Spain
[b] Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, E-28049 Madrid, Spain
[c] Instituto Nicolás Cabrera (INC), Universidad Autónoma de Madrid, E-28049 Madrid, Spain.

* lucia.romeros@estudiante.uam.es

2D materials have revolutionized current research [1]. In particular, the ability to stack them at defined angles has unlocked an endless reservoir of novel materials. This angle control—often referred to as "twistronics"—enables unprecedented tuning of electronic, optical, and mechanical properties, fostering the emergence of exotic quantum phenomena such as correlated electron behavior and unconventional superconductivity. A paradigmatic example of this exciting phenomena are twisted bilayer graphene devices rotated at magic angles [2-3]. A current yet unsolved challenge is to address both macroscopic and atomic scale properties at the same time. In order to combine both worlds, our group has recently developed an UHV-LT-STM/AFM system that can also perform in situ transport measurements. With the system perfectly optimized, now we face a key challenge: the need of atomically clean 2D devices. Here, we present the experimental tools we have developed to prepare and efficiently characterize twisted 2D devices. We have developed a new transfer system to prepare twisted 2D devices precisely, which we are currently using to investigate twisted graphene devices at the magic angle. In combination, we have also developed an UHV-RT-AFM/STM setup, compatible with in-situ transport measurements, to study of both macroscopic and microscopic properties in a very efficient way. Its main objective is to allow a fast inspection, characterization and manipulation of 2D devices. In this work, we present both, transfer and AFM systems, and the preliminary experimental results

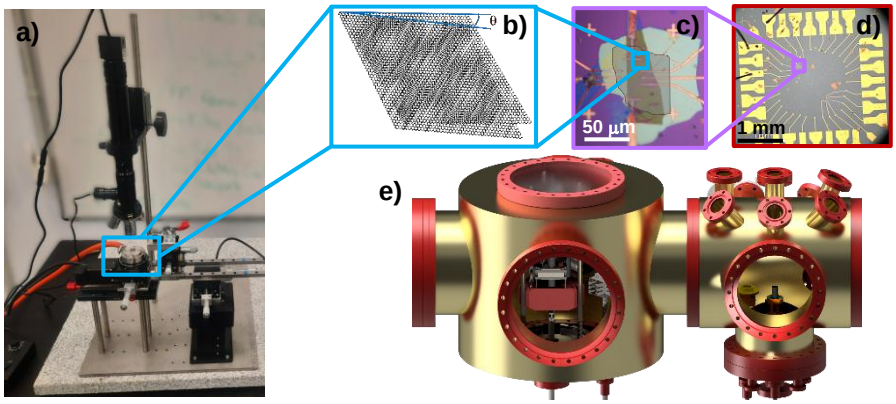

Figure: a) Transfer system for twisted devices preparation. Its main features are motorized vertical and angular stages, which allow us to precisely control the rotation angle between layers (b). c-d) After stacking, the device is then mounted to a sampleholder for its characterization. e) 3D design of the UHV-RT-AFM/STM equipment. The system includes a main chamber, which contains the microscope, and a preparation chamber

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Spin and charge control of topological end states in chiral graphene nanoribbons

Leonard Edens[1] , Francisco Romero Lara[1] , **Trisha Sai[1]** , Kalyan Biswas[1] , Manuel Vilas-Varela[2] , Sofia Sanz[3] , Thomas Frederiksen[4] , Fabian Schulz[1] , Diego Peña[2] , and Nacho Pascual[1]

[1] CIC nanoGUNE BRTA, Donostia-San Sebastián, Spain
[2] CiQUS and Universidade de Santiago de Compostela, Spain
[3] CFM, Donostia-San Sebastián, Spain
[4] DIPC, Donostia-San Sebastián, Spain

t.sai@nanogune.eu

Atomic monolayers of rare earth-noble metal alloys exhibit interesting structural and magnetic properties. Here, we exploit these properties by using these materials as substrates to study graphene nanostructures. We prepare GdAu2 by depositing Gd onto a hot Au(111) crystal[1]. As for the case of Au(111), $GdAu_2$ also catalyses the synthesis of (3,2,8)-chiral nanoribbons (chGNRs)[2]. Using a low temperature Scanning Tunneling Microscope (STM), we observed that the spins at the topological end states of these chGNRs are not quenched by charge transfer with the substrate, in contrast to previous observations on other substrates[3]. This opens up the possibility of studying their magnetic properties.

We identify two different classes of chGNRs. Depending on the occupancy of the two topological end states, they are either neutral or anionic (Figure 1). We show that we can switch from single to double occupancy by lateral manipulation of the chGNR along the substrate's moiré lattice using the STM tip. These changes in occupancy are attributed to the variation of the local work function of the substrate. The redistribution of charge is verified by Kelvin probe force microscopy (KPFM). Further, the chGNRs experience a magnetic field (B_{eff}), which arises as a result of the exchange bias between the chGNRs and the ferromagnetic substrate[4]. This B_{eff} manifests as low energy inelastic features in STS, which are interpreted as Kondo screened spin-flip excitations of the π radical site.

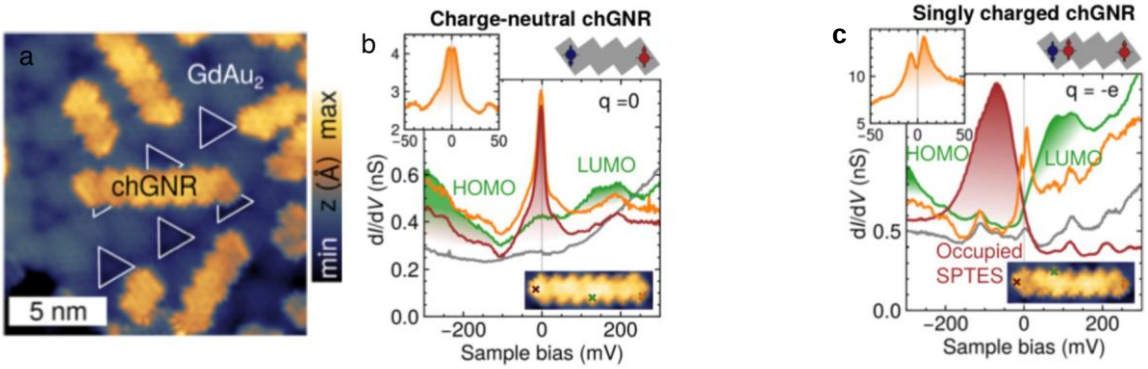

Figure 1: a) STM scan of chGNRs directly synthesized on the GdAu2 surface. b) STS of charge neutral chGNR with a Kondo peak split. c) STS of singly charged (anionic) chGNRS, with an occupied orbital on one end, and a Kondo peak split on the other.

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Concavity vs convexity: the role of molecular configuration on the reaction pathway

F. Villalobos,[a,b] J. I. Mendieta-Moreno,[b] J. Lobo-Checa,[c] S. P. Morcillo,[a] J. M. Gómez-Fernández,[b] P. L. de Andrés,[b] J. I. Martínez,[b] J. A. Martin-Gago,[b] J. M. Cuerva,[a] A. G. Campaña,[a] **C. Sánchez-Sánchez[b*]**

[a]*Departamento de Química Orgánica, Universidad de Granada (UGR), Unidad de Excelencia de Química UEQ, C. U. Fuentenueva, 18071 Granada, Spain.*
[b]*ESISNA Group, Instituto de Ciencia de Materiales de Madrid (ICMM-CSIC), Sor Juana Inés de la Cruz 3, 28049 Madrid, Spain.*
[c]*Instituto de Nanociencia y Materiales de Aragón (INMA), CSIC−Universidad de Zaragoza, Zaragoza 50009, Spain; Departamento de Física de la Materia Condensada, Universidad de Zaragoza, Zaragoza 50009, Spain*

* cssanchez@icmm.csic.es

The role of stereochemistry—the spatial arrangement of atoms within molecules—on the reaction pathway of organic molecules has been largely overlooked in on-surface synthesis despite being crucial in organic chemistry. In this work, we demonstrate how the starting diastereomeric configuration can drive the adatom-induced transformation of a substituted cyclooctatetraene (COT) structure—a key molecule in the study of aromaticity—into a cyclopenta[c,d]azulene (CPA) structure, within a chevron-shaped graphene nanoribbon (GNR) [1]. Remarkably, the predominant product, the CPA chevron-like GNR, displays the lowest bandgap ever recorded for an all-carbon chevron-shaped GNR. This research opens up new possibilities for applying stereochemical principles in the design of innovative graphene-based nanostructures.

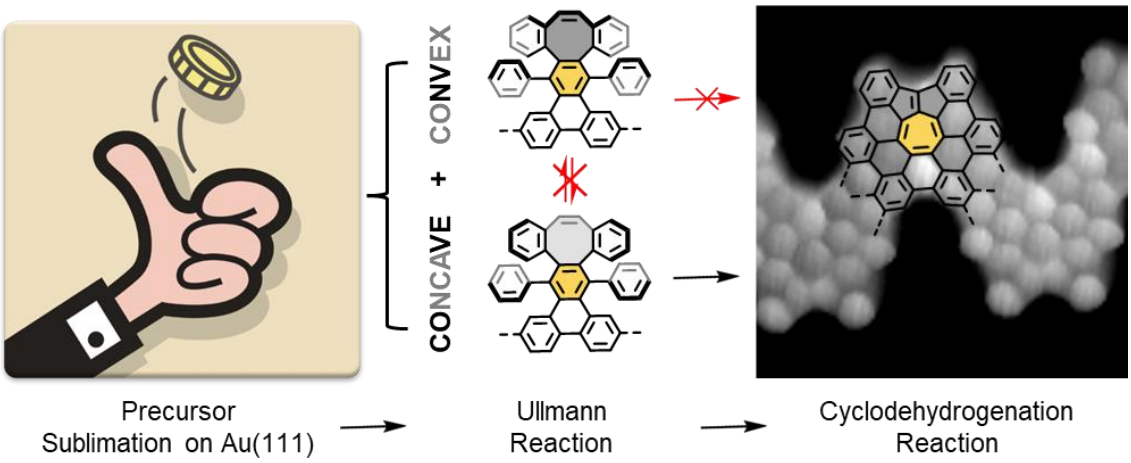

Figure – Schematic representation of the process and bond-resolved STM image of the final CPA-GNR.

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Atomically Resolved Magnetic Structure of Rare Earth Gold Surface Alloys

E. Peláez-Sifonte [a], A. Moya-Señas [a], J. Brede [b], L. Fernández [b], F. Romero-Lara [c], F. Schiller [b], J. Lobo-Checa [a], **D. Serrate** [a,d]

[a] Instituto de Nanociencia y Materiales de Aragón, CSIC-Universidad de Zaragoza, Zaragoza, Spain
[b] Centro de Física de Materiales, CSIC-UPV, San Sebastián, Spain
[c] CIC-NanoGUNE-BRTA, San Sebastián, Spain
[d] Laboratorio de Microscopias Avanzadas, Universidad de Zaragoza, Zaragoza, Spain

* serrate@unizar.es

$REAu_2$ (RE=rare earth) alloys on Au(111) can grow as a monolayer thick ferromagnetic 2D film. Furthermore, the mismatch between the alloy lattice parameter and the underlying Au(111) structure gives rise to a surface reconstruction forming a superstructure with a pitch of the about 3.5 nm. These surfaces have aroused remarkable interest following the demonstration of similar catalytic properties to bare Au(111) for on-surface synthesis [1]. When varying the RE atom, the number of electrons on the 4f-shell and the interaction with the outer orbitals determine the magnetocrystalline anisotropy and the transition temperature, as disclosed by spatially averaging techniques like X-ray circular dichroism [2] and Kerr effect. Upon closer inspection by spin-polarized STM, $GdAu_2$ revealed an intricate checkerboard arrangement of the magnetic domains at the nanoscale [3]. In this work, we have applied the SP-STM technique to several of these alloys (RE=Gd, Ho, Tb, Eu) and imaged the spin density with atomic resolution as a function energy (range of ±3 eV) and out-of-plane magnetic field. We find that the appearance of structural antiphase domain boundaries (APB, atomically sharp crystalline defects caused by the relative shift of the unit cell at both sides) determines the magnetic properties of the ferromagnetic monolayers to a great extent. In particular, in $GdAu_2$ with strong in-plane magnetic anisotropy, APB fronts at 60 º from the lattice shift vector produce strong antiferromagnetic coupling among the structural domains at either side of it. On the other hand, HoAu2 and TbAu2 with out-of-plane magnetic anisotropy display the same type of structural domains, but no spin-polarized states have been detected by our SP-STM probe spilling out into the vacuum. Finally, $EuAu_2$ displays out-of-plane spin contrast with no traces of structural APBs.

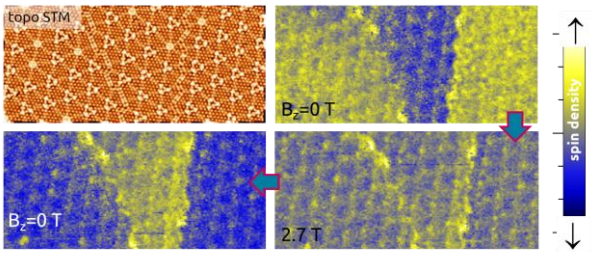

Figure – Simultaneous STM topography image (U=-1 V) and spin resolved tunneling conductancs (U=3 V) taken with a Cr in-plane sensitive tip. The two images at zero field represent opposite remanent states achieved after out-of-plane saturation above 2.7 Tesla.

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Magnetic Nanoparticles for Biomedical Applications

Jorge A. L. Solaiman[a], Célia T. Sousa[b] , Agustina Asenjo [a], Eider Berganza[a].

[a] Instituto de Ciencias de Materiales de Madrid, CSIC.
[b] Universidad Autónoma de Madrid

* jorgea.lopez@icmm.csic.es

Research on magnetic nanostructures has become one of the most interesting areas in recent years for the development of nanotechnology [1]. This work explores nanofabrication routes for active surfaces aimed at cellular stimulation, based on magnetic Janus nanoparticles (NPs) and nanodiscs. The Janus NPs are fabricated through a combination of Langmuir-Blodgett technique, which forms self-assembled silica NP monolayers [2], with physical vapor deposition methods to add a magnetic coating (Terfenol-D) Furthermore, nanodiscs are fabricated through Hole Mask Colloidal Lithography with the goal of preparing nanostructures with the same material but different geometries.

Magnetic characterization techniques, such as vibrating sample magnetometry (VSM) and magnetic force microscopy (MFM), have been employed to understand the magnetic response of our nanostructured surfaces to external stimuli. Cell viability experiments have been conducted using two types of living human cells. On one hand, astrocytes have been used to study the cytotoxicity of Terfenol-D, while glioblastoma cells have been used to analyze the stimulation capacity via magnetostrictive effects of structures coated with the mentioned material [3]

The results obtained demonstrate the effectiveness of the Langmuir-Blodgett technique for the fabrication of compact monolayers (see Figure). Moreover, the effects of nanostructuration on magnetic properties have been determined. Finally, magnetic field-induced cell stimulation has been shown to influence cell population dynamics.

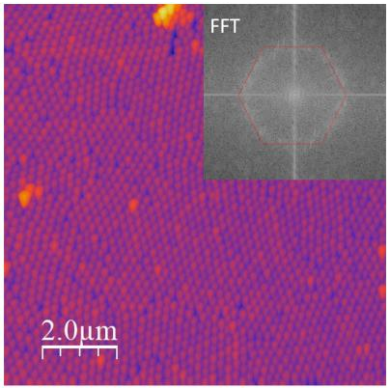

Figure - Monolayer of 200 nm silica NPs obtained via Langmuir-Blodgett technique alongside the corresponding Fourier transform, underlined to see the hexagonal symmetry.

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Using Machine Learning to quantify how molecular structural variables change the conductance of single molecule junctions

H. Vázquez [a]

[a] Institute of Physics, Czech Academy of Sciences, Cukrovarnická 10, Prague 16200, Czech Republic

* vazquez@fzu.cz

In single molecule electronics, where individual molecules are placed between two nanoscale electrodes, conductance depends critically on the geometry at the junction. During STM break-junction experiments, molecular geometry is believed to change significantly since measurements are often carried out at room temperature. Our aim is to quantify the effect on conductance of these changes in molecular conformation. DFT-NEGF simulations are ideally suited to address this, but their computational cost restricts limits them to only a few junction geometries.

We use a recently developed computationally efficient method to calculate molecular conductance within DFT for thousands of geometries, based on small Au-molecule-Au clusters [1,2]. We perform MD simulations of the junction at room temperature, from which we sample the geometries adopted by the molecule. We then calculate the junction conductance of these thousands of geometries. This allows us to compute the variation in conductance arising from thermally-induced conformational changes.

We use machine-learning methods including regression models and SHAP values to identify which of the bond lengths, angles, or dihedral angles in the molecule, all of which are changing continuously and simultaneously during the MD simulations, have a greater impact on conductance. We apply these techniques to study a series of amine-bonded oligophenyls of different lengths. Our work elucidates how molecular conformational changes contribute to the width of the conductance signal in single molecule junctions.

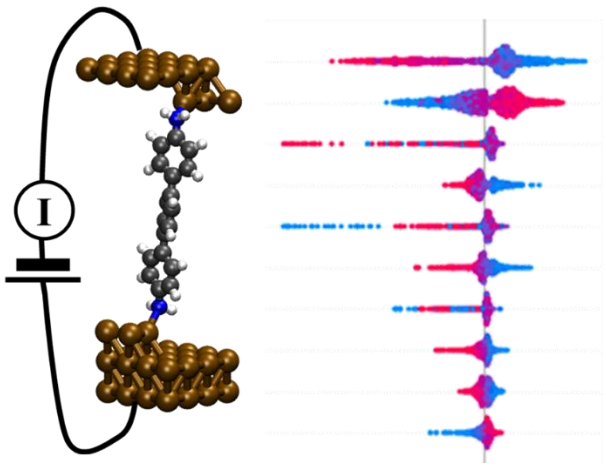

Figure – Schematic of a single molecule circuit and calculated SHAP values of the different structural parameters.

References

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Energy dissipation at a single molecule level

A.M. Zamora-Vinaroz [a,b,*], O. Gutierrez-Varela [a,c], J. J. Mazo [b], and J.G. Vilhena [a]

[a]Materials Science Institute of Madrid, Spanish National Research Council, 28049 Madrid, Spain
[b]Dept. of Structure of Matter, Thermal and Electronic Physics, Univ. Complutense of Madrid, 28040 Madrid, Spain
[c]Departamento de Física Teórica de la Materia Condensada, Facultad de Ciencias, Univ. Autónoma de Madrid, Spain

*azamora@ucm.es

On-surface synthesis provides precise control over nanostructure formation and material composition by confining reactants to two dimensions, enabling the creation of otherwise unattainable molecular compounds [1]. This method is especially useful for atropisomers—molecules with restricted torsional rotation around a single bond. Exfoliation studies have explored the mechanical and tribological properties of surface-synthesized polyaromatic hydrocarbon chains, primarily using Scanning Probe Microscopy under cryogenic conditions and Molecular Dynamics (MD) simulations [2,3]. However, the mechanisms governing energy dissipation during nanomanipulation—specifically, the lifting and redeposition processes—remain unclear. In this work, we address this gap by combining MD simulations, employing a tailored force field, with Atomic Force Microscopy (AFM) experiments using a tuning fork sensor in ultra-high vacuum and cryogenic conditions. Our focus is on the exfoliation of class 1 atropisomeric molecules, an elusive molecular compound. Preliminary results reveal periodic drops in the frequency shift during the lifting and redeposition processes, which are associated with the desorption and adsorption of monomers on the surface—consistent with previous studies [2,3]. Interestingly, the periodicity of these frequency shift drops is shorter than the monomer size, associated to a tethering effect. Furthermore, for the first time, we not only measure the force and its gradient but also quantify the energy dissipated during the exfoliation of a single molecule. We explore different scenarios by analyzing dissipation properties under various conditions, such as distinct stereochemical conformations and varying rigidity of the tethering point. These findings have important implications for emerging fields in nanotechnology and materials science, including nanoelectronics and molecular motors.

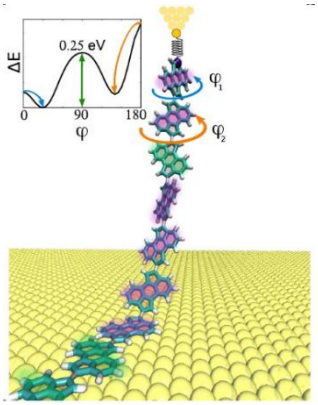

Figure – MD snapshot of the desorption process of sterically frustrated CPAA conformers. The torsion angles of the first two units after detachment are highlighted.

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Tuesday	Wednesday	Thursday	Friday
Arrival in Oviedo FUERZAS Y TÚNEL	**9:00 Key: Jeppe Lauritsen** 9:45 S. Jiménez-Fernández 10:00 K. García Diez 10:15 J. Redondo 10:30 A. Sáez-Coronado	**9:00 Key: Wouter H. Roos** 9:45 A. Díez-Martínez 10:00 E. M. Martín-Cuevas 10:15 B. Cantero-Nieto 10:30 M. Grabarics	**9:00 Key: Laura Fumagalli** 9:45 J. Hwan-Jeong 10:00 P. Sudersan 10:15 D. Martin-Jimenez 10:30 I. Horcas
	10:45 Coffee Break	10:45 Coffee Break	10:45 Coffee Break
	11:15 E. Osuna **11:30 Borja Cirera** 12:00 M. Varea 12:15 A. Pinar-Solé 12:30 B. Mallada 12:45 B. Lowe	11:15 M. Cano **11:30 Yu Kyoung Ryu** 12:00 A. Zambudio 12:15 B. Viña-Bausá 12:30 D. Expósito 12:45 H. González-Herrero	**11:15 Ana Sánchez-Grande** 11:45 E. Tosi 12:00 S. Salaverría 12:15 F. Villalobos 12:30 E. Peláez-Sifonte 12:45 K. Biswas
	13:00 Lunch	13:00 Lunch	**13:00 Concluding Remarks**
	14:30 Ana Pérez 15:00 E. Calle 15:15 P. Martinez-Outomuro 15:30 J. Marqués-Marchán 15:45 D. A. Aldave	**14:30 A. J. Martínez-Galera** 15:00 O. Gutiérrez-Varela 15:15 K. Kim 15:30 M. González-Lastre	
	16:00 Coffee Break	15:45 *LMA* 15:55 *SPECS* 16:05 *OMICRON* 16:15 *RHK* 16:25 *SCIENTEC IBERICA*	
	16:30 M. Navarro-Rodríguez 16:45 D. Gallego-Fuente **17:00 Carlos Romero-Muñiz** 17:30 A. Gallardo 17:45 J. Trujillo-Mulero 18:00 O. Mateos-Lopez	**16:40 – 19:00** **Poster session / Coffee Break**	
18:00 Registration			
18:30 **Opening** 19:00 **Key: Pablo Alonso**			
20:00 Welcome cocktail		20:00 Conference Dinner	