

# jsi2024 : Journées surfaces & interfaces

24-26 janv. 2024 Grenoble (France)

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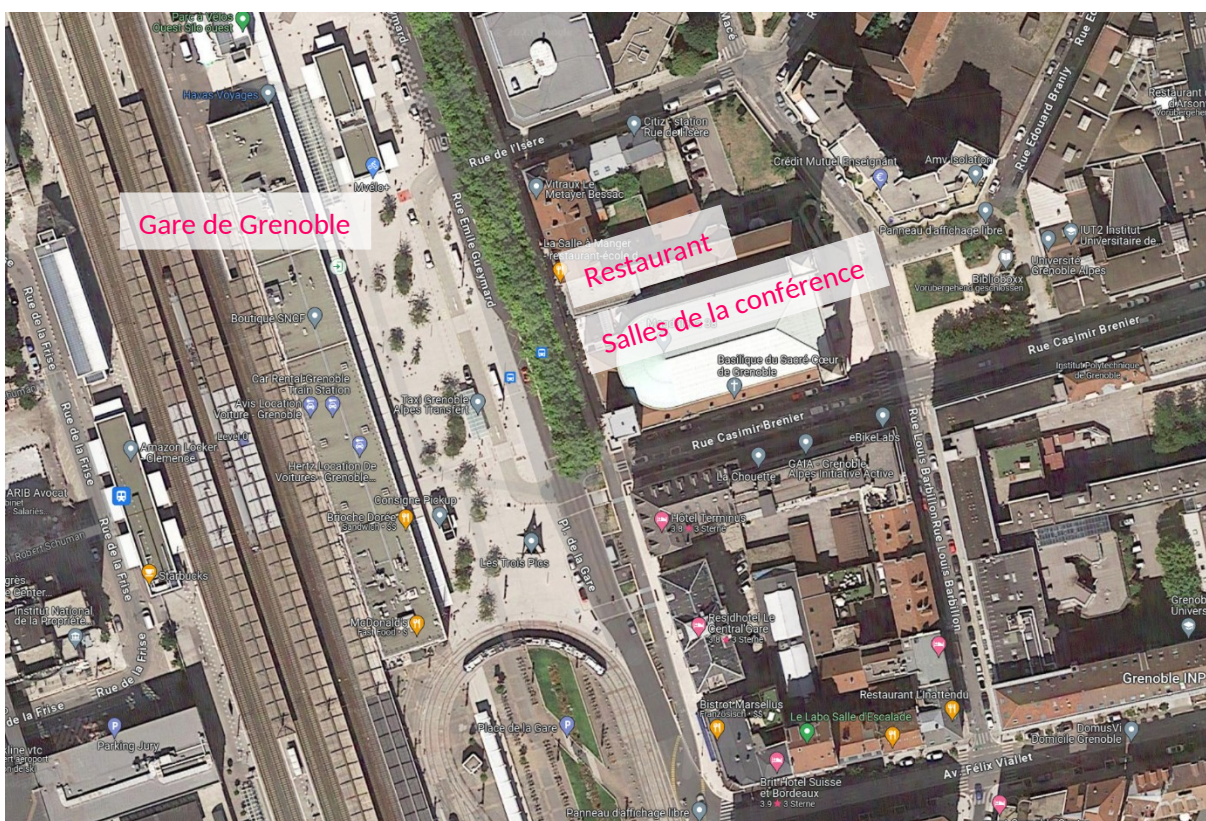
## Exposants



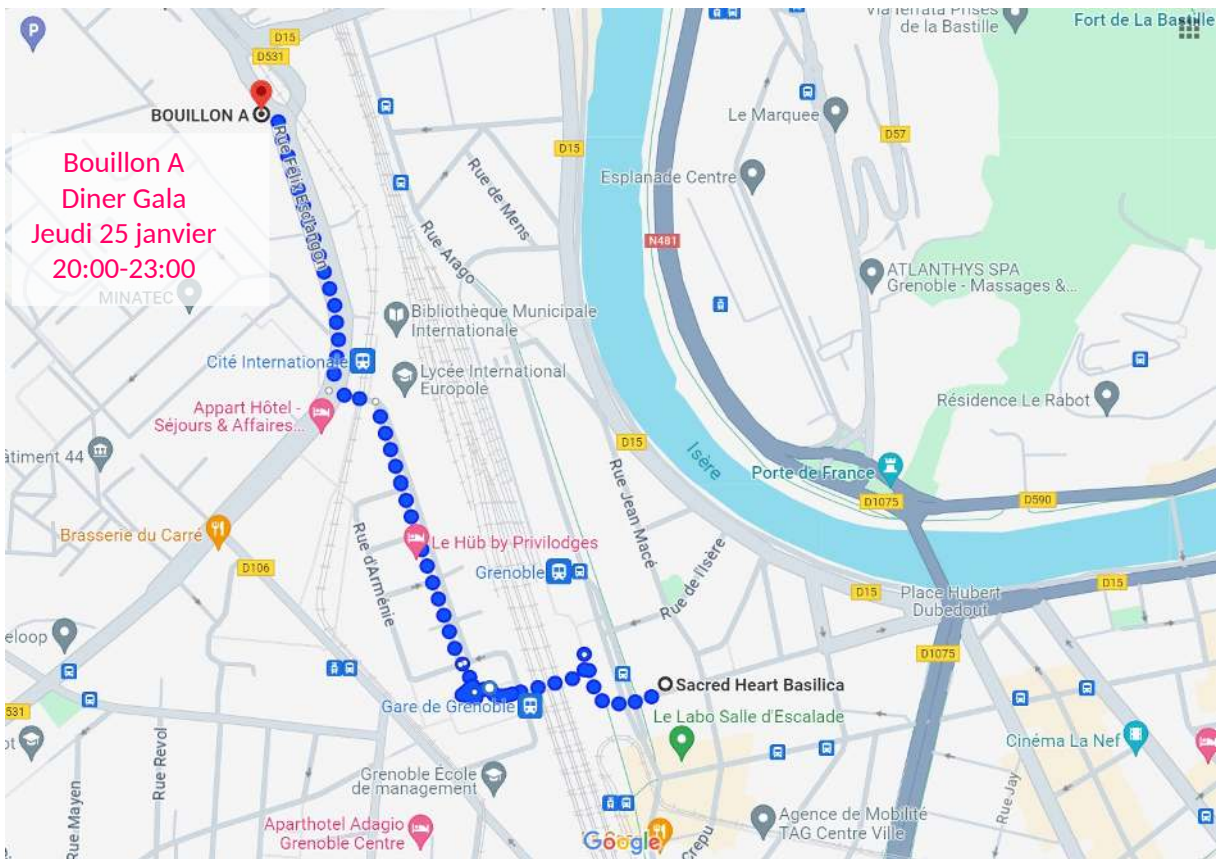
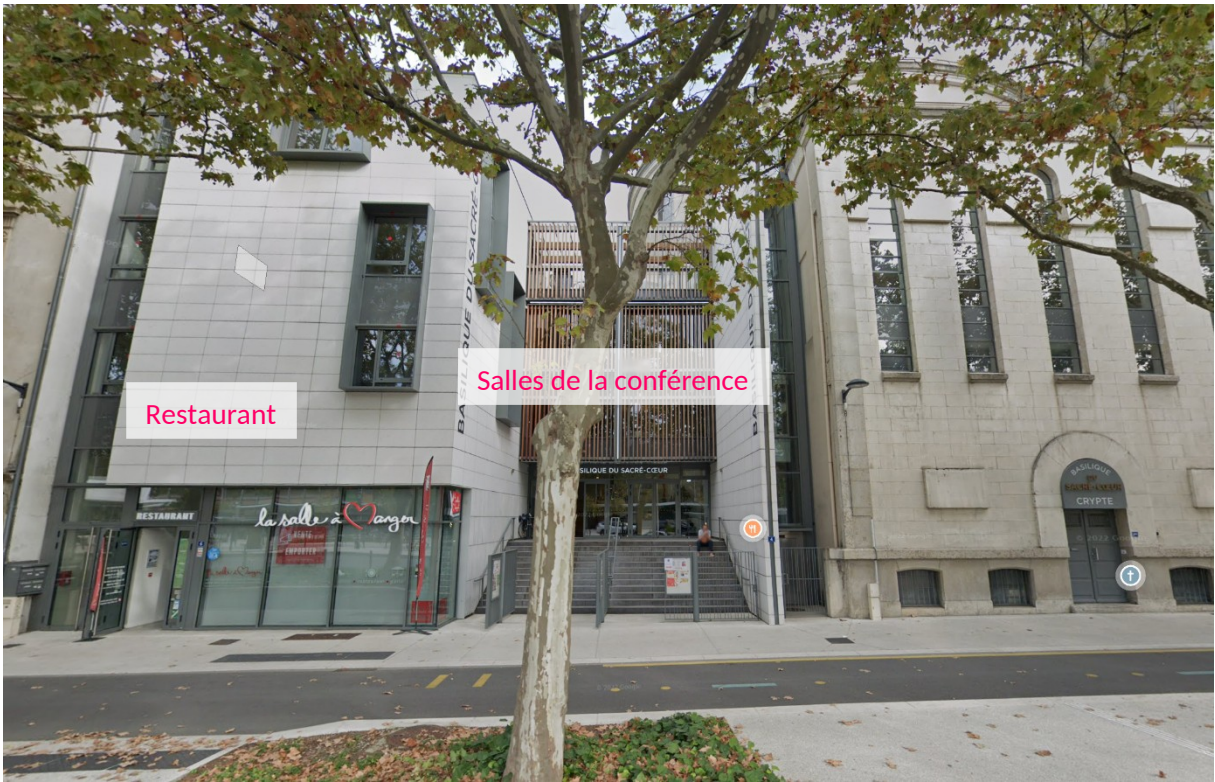
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## Les Lieux







## Mercredi 24 janvier 2024

09:00 - 10:15 Accueil des participantes et participants

10:15 - 10:30 Ouverture des JSI - Comité d'organisation – **AUDITORIUM**

### Thématique élargie – **AUDITORIUM**

10:30 - 11:15 › Composition and degradation of artworks revealed by synchrotron-based X-ray microscopies - **Marine Cotte**, *European Synchrotron Radiation Facility, Laboratoire d'Archéologie Moléculaire et Structurale*

### Nanoparticules, catalyse – **AUDITORIUM**

11:15 - 12:00 › Synthesis of metal nanoparticles by an organometallic route and applications in catalysis - **Karine Philippot**, *Laboratoire de chimie de coordination*

### Matériaux 2D – **AUDITORIUM**

12:00 - 12:45 › Berry Curvature Signatures in Dichoic Photoemission and Chiroptical Excitonic Transitions - **Samuel Beaulieu**, *Université de Bordeaux - CNRS - CEA, CELIA*

12:45 - 14:00 Déjeuner – **RESTAURANT SALLE À MANGER**

### Magnétisme – **AUDITORIUM**

14:00 - 14:45 › Chiralité magnétique aux interfaces : l'interaction de Dzyaloshinskii-Moriya - **André Thiaville**, *Laboratoire de Physique des Solides, Université Paris Saclay, 91405 Orsay, France*

### Croissance, épitaxie – **AUDITORIUM**

14:45 - 15:30 › Atomic Layer Deposition for photovoltaic applications - **Nathanaelle Schneider**, *Institut Photovoltaïque d'Ile-de-France (ITE), Institut Photovoltaïque d'Ile-de-France (UMR IPVF 9006)*

15:30 - 16:00 Pause café – **ESPACE PIANO**

### Matière molle – **AUDITORIUM**

16:00 - 16:45 › Shear-thickening in presence of adhesive contact forces: the singularity of cornstarch - **Anaïs Gauthier**, *Institut de Physique de Rennes*

16:45 - 17:30 › Coated microbubbles exploit shell buckling to swim - **Gwennou Coupier**, *Laboratoire Interdisciplinaire de Physique [Saint Martin d'Hères]*

17:30 - 18:15 › Watching single charge transport at liquid/solid interfaces - **Jean Comtet**, *Laboratoire Sciences et Ingénierie de la Matière Molle*

## Jeudi 25 janvier 2024

### Thématique élargie – AUDITORIUM

08:30 - 09:15 › Champagne! The science behind the bubble - **Gérard Liger-Belair**, Groupe de spectrométrie moléculaire et atmosphérique

### Magnétisme – AUDITORIUM

09:15 - 10:00 › Controlling magnetism by ionic liquid gating - **Liza Herrera-Diez**, Centre de Nanosciences et de Nanotechnologies

### Croissance, épitaxie – AUDITORIUM

10:00 - 10:45 › 2D oxides: templates for oxide thin films grown by pulsed laser deposition - **Valérie Demange**, Institut des Sciences Chimiques de Rennes

10:45 - 11:15 Pause café – ESPACE PIANO

### STM, transport, optique – AUDITORIUM

11:15 - 12:00 › From quantum dot to infrared imaging - **Emmanuel Lhuillier**, CNRS - Sorbonne Université

12:00 - 12:45 › Building and characterizing artificial III-V lattices for quantum simulations - **Bruno Grandidier**, IEMN, Lille

12:45 - 13:30 Déjeuner – RESTAURANT SALLE À MANGER

13:30 - 15:30 Session poster – ESPACE PIANO

### Hétérostructures – AUDITORIUM

15:30 - 16:15 › Light experiments with infinite-layer nickelates - **Daniele Preziosi**, Institut de Physique et Chimie des Matériaux de Strasbourg

16:15 - 17:00 › Lumière sur les matériaux ferroélectriques: films minces épitaxiés et microdispositifs - **Sylvia Matzen**, Centre de Nanosciences et de Nanotechnologies CNRS, Paris-Saclay University [Orsay]

17:00 - 17:45 › Coupling of metal-insulator transitions in nickelate based superlattices - **Jean-Marc Triscone**, Department of Quantum Matter Physics [Geneva]

20:00 - 23:00 Dîner de gala – LE BOUILLON A

## Vendredi 26 janvier 2024

### Thématique élargie - AUDITORIUM

09:00 - 09:45 › Using magnetism to act on living cells - **Bernard Dieny**, *SPINtronique et TEchnologie des Composants*

### Matériaux 2D

09:45 - 10:30 › The art of seeing electrons and playing with their spins - **Federico Mazzola**, *University of Ca' Foscari [Venice, Italy], CNR, Italian national research Center*

10:30 - 11:00 Pause café

### Matériaux 2D - AUDITORIUM

11:00 - 11:45 › L'eau comme source de charge ou comme ligand aux interfaces liquide-solide - **Marie-Laure Bocquet**, *Laboratoire de physique de l'ENS - ENS Paris*

11:45 - 12:30 › Modelling electronic transport in 2D materials - **Thibault Sohier**, *Laboratoire Charles Coulomb*

12:30 - 12:45 Fermeture des JSI - Comité d'organisation, comité scientifique

12:45 - 14:00 Déjeuner - **RESTAURANT SALLE À MANGER**

(ou à emporter si choisi)

# Présentations

24 janvier 2024



# Composition and degradation of artworks revealed by synchrotron-based X-ray microscopies

M. Cotte<sup>1,2</sup>

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The application of analytical chemistry to study artworks has been intensely increasing over the last decades and tackle questions ranging from production to degradation processes of cultural heritage objects. Synchrotron techniques can offer detailed information to help answer these questions by deciphering the material composition and structure. In 2020, the ESRF was upgraded to become the ESRF-EBS (Extremely Brilliant Source), resulting in an increased brightness and coherence of the synchrotron beam, paving the way to cutting-edge analytical capacities. Besides, continuous developments of beamline instrumentations boosted their speed and efficiency.[1] The micro-spectroscopy beamline ID21 has long been used for heritage science and will be even more with the refurbishment of the beamline and the installation of a new nano-scope. The heritage community is also increasingly using the diffraction beamlines ID13 and ID22 through a facilitated access, the historical materials “BAG” (block allocation group) [2]. Synchrotron-based X-ray microscopes allow tackling the matter composition in the different parts of the objects, and in particular assessing chemical modifications between the bulk layers (original) and the degraded surface. Species and crystalline phases can be not only identified but also located, giving clues about the artist's techniques as well as the conservation state of the artwork. The talk will be illustrated by different recent works. [3, 4]

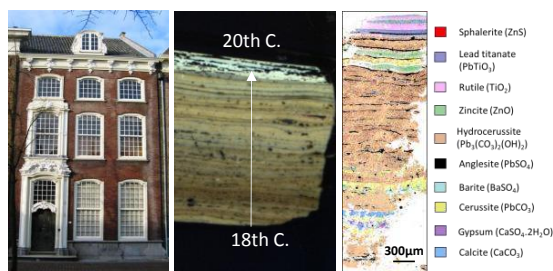


Fig.1. Micro X-ray diffraction ( $\mu$ XRD) mapping of a fragment of paint from wood frames of De Witte Roos in Delft: the map reveals the evolution of lead paint composition from the 18<sup>th</sup> to the 20<sup>th</sup> C but also their degradation ( $\text{PbSO}_4$ ) [5].

[1] M. Cotte, K. Dollman, V. Fernandez, V. Gonzalez, F. Vanmeert, L. Monico, C. Dejoie, M. Burghammer, L. Huder, S. Fisher, W. de Nolf, I. Fazlic, H. Castillo-Michel, M. Salomé, M. Ghirardello, D. Comelli, O. Mathon and P. Tafforeau, *SRN* **35** (5), 1-7 (2022).

[2] M. Cotte, et al., *Molecules* **27**, 1997 (2022).

[3] V. Gonzalez, M. Cotte, G. Wallez, A. van Loon, W. de Nolf, M. Eveno, K. Keune, P. Noble and J. Dik, *Angew Chem*, **58** (2019).

[4] V. Gonzalez, G. Wallez, E. Ravaud, M. Eveno, I. Fazlic, T. Fabris, A. Nevin, T. Calligaro, M. Menu, V. Delieuvin and M. Cotte, *JACS*, (2023).

[5] S. Hageraats, M. Thoury, M. Cotte, L. Bertrand, K. Janssens and K. Keune, in *Analytical Chemistry for the Study of Paintings and the Detection of Forgeries*, ed. M. P. Colombini, I. Degano and A. Nevin, Springer International Publishing, Cham. (2022), pp. 359-418.



# Synthesis of metal nanoparticles by an organometallic route and applications in catalysis

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Owing to their attractive properties and potential applications in various fields, a great deal of effort is being devoted to the design of metal nanoparticles (MNPs). The 'Metal Nanoparticle Engineering' team at the LCC-CNRS (Toulouse, France) has developed an effective toolbox for the synthesis of controlled MNPs using molecular chemistry concepts. This approach relies on the hydrogenation of organometallic or metal-organic complexes under mild conditions (room temperature; 3 bar H<sub>2</sub>) in the presence of ligands as stabilizing agents [1]. It allows to obtain MNPs of small size (<10 nm) and controlled composition, monometallic or bimetallic (alloy, core-shell, surface-decorated). These nanoparticles can be deposited on a support by simple impregnation or by direct synthesis in the presence of the chosen support (polymers, ionic liquids, silica, alumina, carbon materials, etc.). These MNP systems are pertinent models for fundamental studies. They also find applications in various fields such as catalysis [2,3]. The valorization of biomass [4,5], the development of catalysts for the production of renewable energy sources, for the production of hydrogen by the process of water separation [6,7] or the valorization of CO<sub>2</sub> [8] are some illustrative recent works.

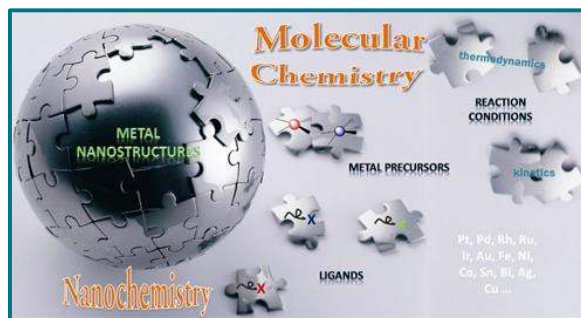


Fig.1. A molecular chemistry toolbox for the synthesis of metal nanoparticles

## References

- [1] C. Amiens, D. Ciuculescu-Pradines, K. Philippot, *Coord. Chem. Rev.*, 38, 409 (2016),
- [2] M. R. Axet, *Chem. Rev.* 2020, *Chem. Rev.* 120, 2, 1085 (2020).
- [3] *Nanoparticles in Catalysis: Advances in Synthesis and Applications*, Wiley-VCH, K. Philippot & A. Roucoux (Eds.), 2021.
- [4] M. Cardona, P. Lecante, C. Dinoi, I. del Rosal, R. Poteau, K. Philippot, M. Rosa Axet, *Green Chemistry*, 23, 8480 (2021).
- [5] L. Bruna, M. Cardona-Farreny, V. Colliere, K. Philippot, M. R. Axet, *Nanomaterials*, 12 (3), 328 (2022).
- [6] J. Creus, S. Drouet, S. Suriñach, P. Lecante, V. Collière, R. Poteau, K. Philippot, J. García-Antón, X. Sala, *ACS Catalysis*, 8, 11094 (2018).
- [7] N. Romero, D. A. Fenoll, L. Gil, S. Campos, J. Creus, G. Martí, J. Heras-Domingo, V. Collière, C. A. Mesa, S. Giménez, L. Francàs, L. Rodríguez-Santiago, X. Solans-Monfort, M. Sodupe, R. Bofill, K. Philippot, J. García-Antón, X. Sala, *Inorg. Chem. Front.*, 10, 5885 (2023).
- [8] X.-P. Fu, L. Peres, J. Esvan, C. Amiens, K. Philippot, N. Yan, *Nanoscale*, 13, 8931 (2021).

# Berry Curvature Signatures in Dichroic Photoemission and Chiroptical Excitonic Transitions

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The topology of the electronic band structure of solids can be described by its Berry curvature distribution across the Brillouin zone. However, experimentally accessing momentum-resolved Bloch electrons' quantum geometry still remains a grand challenge. In this talk, I will present new approaches based on different flavors of angle-resolved photoemission spectroscopy, that allow access to robust signatures of local Berry curvature in the paradigmatic transition metal dichalcogenide  $WSe_2$ .

In the first approach [1], we combined circular dichroism, photon-energy-dependent, and nano-ARPES at the I05 beamline (Diamond Light Source) to extract doubly differential photoemission signals that exhibit robust signatures of Berry curvature at the K and K' points of  $WSe_2$ . This measurement methodology seems to be much more resilient than conventional circular dichroism to spurious effects related to experimental geometry and final state effects.

In the second approach [2], we theoretically introduce and experimentally demonstrate a general methodology based on time-resolved ARPES, allowing measuring energy- and momentum-resolved optical transition rates, which can be linked to the Berry curvature texture in reciprocal space. Indeed, by performing time-resolved ARPES of atomically thin  $WSe_2$  using polarization-modulated resonant excitations, we demonstrate that excitons become an asset in extracting the quantum geometrical properties of solids. We also investigate the resilience of our measurement protocol against ultrafast scattering processes following direct chiroptical transitions. These new methods represent a major step forward in going beyond band structure mapping using ARPES [3-6] and can be extended to probe ultrafast modification of materials' quantum geometry during non-equilibrium topological phase transitions [7], for example.

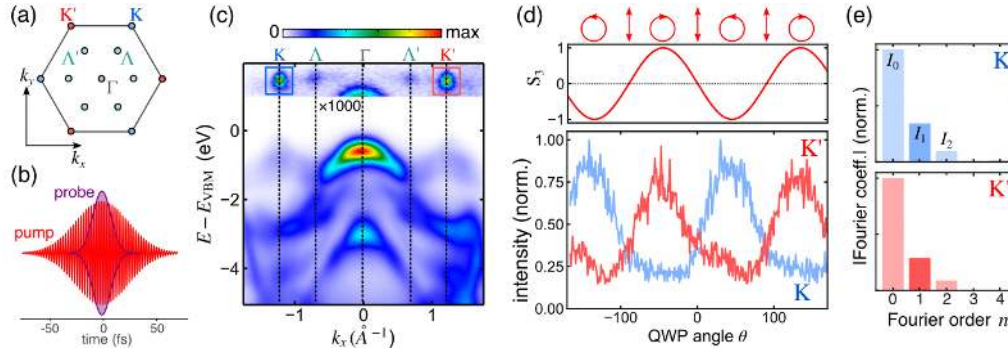


Fig.1. Optical polarization-modulated pump-probe photoemission in monolayer  $WSe_2$ . (a) Sketch of the Brillouin zone of  $WSe_2$  with the high-symmetry points. (b) Sketch of the overlapping pump and probe pulses. (c) Optical polarization-averaged trARPES signal along  $k_x$ . (d) Ellipticity factor of the pump pulse, along with the ellipticity-resolved photoemission intensity of excited states around the K and K' points. (e) The absolute value of the Fourier coefficients associated with the polarization-modulated photoemission intensities from excitonic states in (d).

- [1] Beaulieu and coworkers, *unpublished*
- [2] Beaulieu *et al.*, arXiv:2308.09634 (2023)
- [3] Schüler *et al.*, Physical Review X 12, 011019 (2022)
- [4] Beaulieu *et al.*, Physical Review Letters 125, 216404 (2020)
- [5] Schüler *et al.*, Science Advances 6, 9 (2020)
- [6] Cho *et al.*, Phys. Rev. Lett. 121, 186401 (2018)
- [7] Schüler and Beaulieu, Communications Physics 5, 164 (2022)

## 2D oxides: templates for oxide thin films grown by pulsed laser deposition

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Functional properties such as ferroelectric, multiferroic or transparent conducting oxide in complex oxide thin films are key components in modern devices. Their properties are related to their orientation and to their structural and microstructural qualities in relation with the crystal growth. Epitaxial films are obtained on single-crystalline oxide substrates (such as SrTiO<sub>3</sub>) that present chemical compatibility and small in-plane lattice parameters mismatch with the film. However, these substrates are expensive and size-limited. On the other hand, direct growth of functional oxides on low-cost substrates with large area as silicon or glass leads to amorphous or polycrystalline films with poor properties. Therefore, introduction of a buffer layer is necessary on such substrates in order to achieve the epitaxial growth of complex oxides. Among other candidates, oxide nanosheets have been identified for several years as seed layers to induce the preferential growth of complex oxides with a high crystalline quality, on several low-cost substrates as silicon, glass, mica, polymers and metallic foils [1,2]. These nanosheets are obtained by exfoliation of layered oxides, as KCa<sub>2</sub>Nb<sub>3</sub>O<sub>10</sub>, K<sub>0.8</sub>Ti<sub>2</sub>O<sub>4</sub>, Na<sub>x</sub>MoO<sub>2</sub> [2]. They possess either 2D square, rectangular or hexagonal lattices, allowing regrowth of [001], [011] and [111] preferentially oriented perovskite oxides. The nanosheets are transferred on low-cost substrates by drop casting methods [3], which allow a high surface coverage of the substrate. As example of epitaxial growth, we will show the possibility to integrate complex oxide perovskites thin films grown by pulsed laser deposition, such as La<sub>0.67</sub>Sr<sub>0.33</sub>MnO<sub>3</sub> [4], KNbO<sub>3</sub> [5] and SrVO<sub>3</sub> [6] on glass, silicon and mica.

[1] M. A. Timmerman, R. Xia, P.T.P. Le, Y. Wang, J.E. Elshof. *Chem. Eur. J.* **26**, 1 (2020)

[2] M. Bayraktar, A. Chopra, F. Bijkerk, G. Rijnders. *App. Phys. Lett.* **105**, 132904 (2014)

[3] Y. Shi, M. Osada, Y. Ebina, T. Sasaki. *ACS Nano.* **14**, 15216 (2020)

[4] A. Boileau, M. Dallochio, F. Baudouin, A. David, U. Lüders, B. Mercey, A. Pautrat, V. Demange, M. Guilloux-Viry, W. Prellier, A. Fouchet. *ACS Appl. Mater. Int.*, **11**, 37302-37312 (2019)

[5] F. Baudouin, V. Demange, S. Ollivier, L. Rault, A.S. Brito, A.S. Maia, F. Gouttefangeas, V. Bouquet, S. Députier, B. Bérini, A. Fouchet, M. Guilloux-Viry. *Thin Solid Films*, **693**, 137682 (2020)

[6] A. Boileau, S. Hurand, F. Baudouin, U. Lüders, M. Dallochio, B. Bérini, A. Cheikh, A. David, Fabien Paumier, Thierry Girardeau, P. Marie, C. Labbé, J. Cardin, M. Guilloux-Viry, W. Prellier, Y. Dumont, V. Demange, A. Fouchet. *Adv. Funct. Mater.* **32** (2022) 2108047

## Atomic Layer Deposition for photovoltaic applications

Nitin Mallik,<sup>1,2</sup> Damien Coutancier,<sup>1,2</sup> Vincent Dufoulon,<sup>1,2</sup> Javid Hajhemati,<sup>1,2</sup> Nao Harada,<sup>1,2</sup> Navid Mouhamad,<sup>1,2</sup> Olivier Fournier,<sup>2</sup> Mirella Al Katrib,<sup>1,3</sup> Frédérique Donsanti,<sup>1</sup> Marion Provost,<sup>1</sup> Muriel Bouttemy,<sup>1,3</sup> Jean Rousset,<sup>1</sup> Philip Schulz,<sup>1,2</sup> Nathanaelle Schneider<sup>1,2,\*</sup>

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Atomic Layer Deposition (ALD): a versatile conformal thin film deposition method with atomic-level control for next-generation PV devices

Photovoltaics are growing rapidly (+30-40% installed volume per year) and are facing many challenges (new usages, 4 to 8 TW capacity by 2050). Hence, academic and industrial communities are developing innovative solar cell architectures involving new materials and interfaces. To build such complicated devices, it is necessary to be able to synthesize nanomaterials with a fine control of the composition, thickness and morphology, under constrained conditions.

In this context, ALD (Atomic Layer Deposition) has emerged as a powerful tool because of its unique advantages that I will illustrate with examples in perovskite (PSC) solar cells. Being a gas-phase deposition method based on sequential, self-limiting surface reactions, it allows the preparation at low temperature and on large areas, of pinhole-free conformal thin-films with excellent reproducibility, accurate and simple control of thickness and material properties. Though PSC have reached very high efficiency levels, it is also accompanied by concerns on long-term stability and open questions about up scaled manufacturing. Innovative ALD-charge transport and encapsulation layers can contribute to circumvent those issues.<sup>[1-3]</sup> All these pave the way toward efficient semi-transparent, flexible and/or tandem systems.

In parallel, I will use those application examples to illustrate our efforts in designing new ALD molecular precursors,<sup>[4]</sup> understanding and controlling the growth of ALD functional materials by innovative in-situ instrumentation and modelisation.<sup>[5,6]</sup>

- [1] N. Mallik, J. Hajhemati, M. Frégnaux, D. Coutancier, T. Ashish, S.-T. Zhang, C. Hartmann, E. Hüsam, A. Saleh, T. Vincent, O. Fournier, R. G. Wilks, D. Aureau, R. F. Duarte, N. Schneider, M. Bär, P. Schulz, *Nano Energy* **2023**, submitted.
- [2] O. Fournier, C. D. Bapaume, D. Messou, M. Bouttemy, P. Schulz, F. Ozanam, L. Lombez, N. Schneider, J. Rousset, *ACS Appl. Energy Mater.* **2021**, *4*, 5787–5797.
- [3] F. J. Ramos, T. Maindron, S. Béchu, A. Rebai, M. Frégnaux, M. Bouttemy, J. Rousset, P. Schulz, N. Schneider, *Sustain. Energy Fuels* **2018**, *2*, 2468–2479.
- [4] P.-A. Pavard, Développement d'une méthode innovante d'identification de précurseurs ALD pour un matériau-cible : cas du sulfure de gallium, Thèse de doctorat, Sorbonne Université, **2021**.
- [5] P. Abi Younes, E. Skopin, M. Zhukush, L. Rapenne, H. Roussel, N. Aubert, L. Khrouz, C. Licitra, C. Camp, M.-I. Richard, N. Schneider, G. Ciatto, N. Gauthier, D. Rouchon, E. A. Quadrelli, H. Renevier, *Chem. Mater.* **2022**, *34*, 10885–10901.
- [6] C. Goehry, N. Schneider, *J. Phys. Chem. C* **2017**, *121*, 5871–5881.



# Phase separation and shear thickening of cornstarch suspensions

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A number of dense particle suspensions experience a dramatic increase in viscosity with the shear stress, up to a solid-like response. This shear-thickening process is understood as a transition under flow of the nature of the contacts – from lubricated to frictional – between initially repellent particles. Most systems are now assumed to fit in with this scenario, which is questionable. Using an in-house pressure sensor array, we provide a spatio-temporal map of the normal stresses in the flows of two shear-thickening fluids: a stabilized calcium carbonate suspension, known to fit in with the standard scenario, and a cornstarch suspension, which spectacular thickening behavior remains poorly understood. We evidence in cornstarch a unique, stable heterogeneous structure, which moves in the velocity direction and does not appear in calcium carbonate. Its nature changes from a stress wave to a rolling solid jammed aggregate at high solid fraction and small gap width. The modeling of these heterogeneities points to an adhesive force between cornstarch particles at high stress, also evidenced in microscopic measurements. Cornstarch being also attractive at low stress, it stands out of the classical shear-thickening frame, and might be part of a larger family of adhesive and attractive shear-thickening fluids.

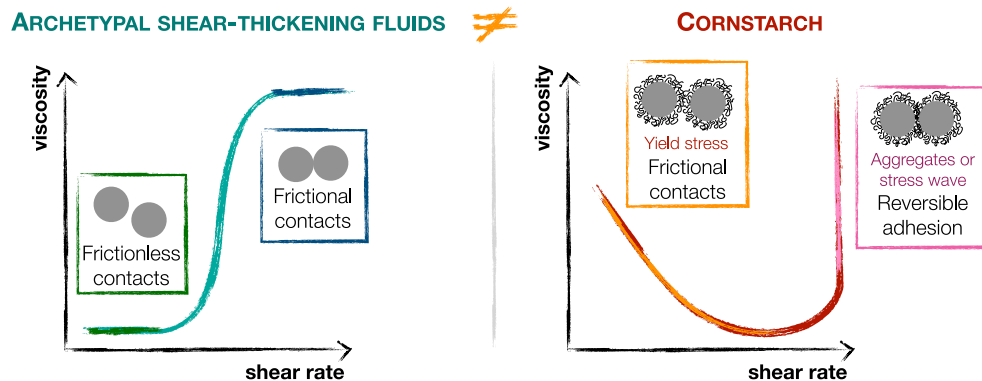


Fig.1. Classical shear-thickening mechanism and suggested mechanism for the shear-thickening of cornstarch suspensions

## Coated microbubbles exploit shell buckling to swim

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The creation of a programmable machine of several microns, capable of carrying out automatically a complex series of actions in our body, was the famous scientific challenge given by Richard Feynman back in 1959 [1]. It was achievable only in science fiction movies (Fantastic Voyage 1966 & Inner Space 1987) until the boom of microrobots research in the past two decades. However, bio-inspired artificial microswimmers share with their natural counterparts an essential flaw: they are slow. Micron-sized swimmers performing shape deformations hardly overcome the 100  $\mu\text{m/s}$  limit. Though inspiration emerging from Nature has led to elegant motility strategies at microscale, this approach contains by itself intrinsic limitations set by the fluid mechanics at this scale, compromising faster displacements. This hinders their use in a complex, crowded and quickly flowing media such as blood, while this would be the main application of such microcargos, that would be able to deliver drugs to specific targets (e.g. tumours).

In our group, we propose to use the deflation-reinflation cycles of an elastic hollow shell submitted to external pressure variations (acoustic wave) to create flow patterns able to quickly propel this shell in a fluid (Fig. 1).

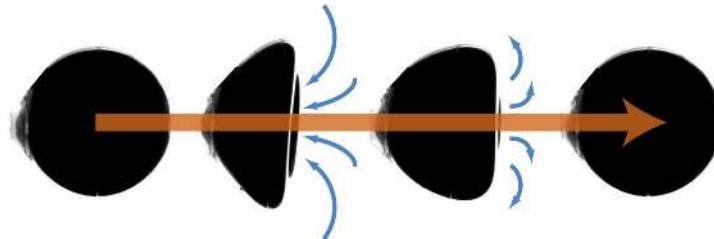


Fig. 1: shell motility activated by pressure; upon an increase of external pressure, a shell suddenly buckles (creation of an inverted cap) and quickly sets a large volume of fluid in motion. If the external pressure is released, the sequence of deformations back to the spherical shape is slower, hence a net displacement of the shell within one pressure cycle [2].

Indeed, soft elastic shells already exist at the microscale. Thin shells (1 – 10 nm) encapsulating tiny gas bubbles (1 – 5  $\mu\text{m}$  in radius) to avoid gas dissolution in the blood plasma are used daily in clinical practice as ultrasound contrast agents (UCAs) and can now be localized in time [3]. The use of UCAs in the medical domain goes beyond imaging; in fact, UCAs can be used as drug carriers [4] whose cargo is released on-demand through ultrasounds at the target site, thereby limiting adverse systemic effects. The release of drug is also obtained by an ultrasonic pulse localized in space and time of sufficient amplitude to break the shell.

Through upscaled experiments, numerical simulations and proof-of-concept demonstrations at the microscale, I will show how these shells, activated by ultrasounds, could also be propelled in a fluid at unprecedentedly reached velocities [5].

[1] R. P. Feynman. There is plenty of room at the bottom: An invitation to enter a new field of physics Miniaturization, Reinhold, 1961.

[2] A. Djellouli, P. Marmottant, H. Djeridi, C. Quilliet, and G. Coupier, Phys. Rev. Lett. **119**, 224501 (2017).

[3] A. Chavignon, B. Heiles, V. Hingot, C. Orset, D. Vivien, and O. Couture, IEEE Transactions on Biomedical Engineering **69**, 2132, 2021.

[4] O. Couture, J. Foley, N. F. Kassell, B. Larrat, and J.-F. Aubry, Transl Cancer Res **3**, 494–511, 2014.

[5] G. Chabouh, M. Mokbel, B. van Elburg, M. Versluis, S. Aland, C. Quilliet, and G. Coupier, Comm. Eng. **2**, 63 (2023).

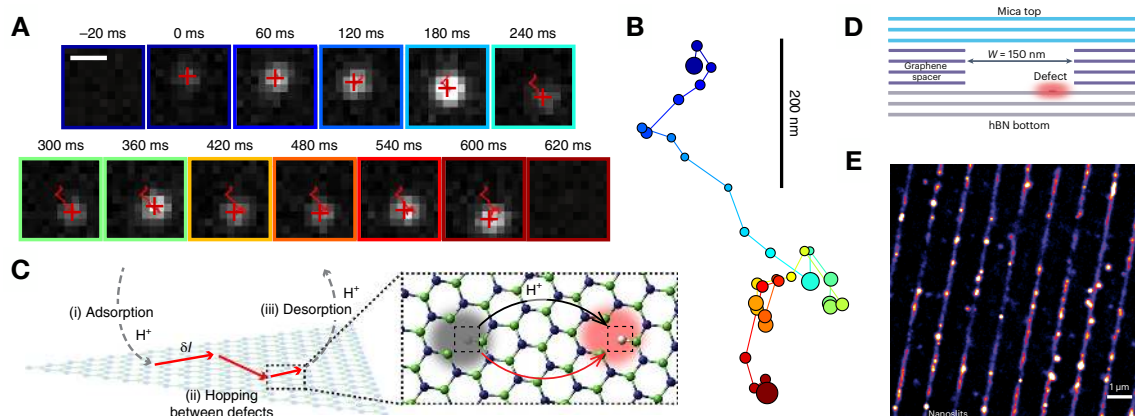
# Watching single charge transport at liquid/solid interfaces

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**Figure.** (A) Time series for spatial migration of luminescence at the surface of the flake. Scale bar, 500 nm. (B) Reconstructed trajectories showing successive activation of adjacent defects at the surface of the flake and colour-coded with increasing time. (C) Schematic depicting luminescence migration events (D) Sketch of the heterostructure nanoslit device. (E) Super-resolved image of acetonitrile-activated emitters embedded in 2.4-nm-high nanoslits.



Understanding the dynamics of charge exchange and transport between a liquid electrolyte and a solid surface is essential for a number of domains, both fundamental (biophysics, nanofluidics, catalysis, electrochemistry...) and applicative (energy storage, energy harvesting, filtration...). However, we remain mostly blind to these interfacial processes, which are currently probed through indirect and ensemble-averaged measurements, hindering their basic understanding.

I will present here recent experimental efforts to resolve interfacial charge dynamics at solid/liquid interfaces at the single-molecule scale, combining Single-Molecule and Super-Resolution microscopy [1] techniques with fluorescent defects hosted in hexagonal Boron Nitride crystals. Starting with aqueous solvents, I will demonstrate how to reveal the trajectories of single proton charges at the interface through the successive activation of ionizable fluorescent surface defects [2]. These observations allowed us to resolve interfacial charge transport with nanometric resolution and over micrometer range, providing experimental evidence at the single molecule scale that interfacial water provides a preferential pathway for lateral charge transport. I will then show the extension of these experiments towards more complex solvents, evidencing the key role of solvent hydrophobicity and charge solvation on interfacial transport [3]. Finally, I will discuss recent efforts to probe the role confinement on molecular charge transport, through careful assembly of van der Waals heterostructures providing slit-like confinement with sub-nanometric control [4].

[1] J. Comtet et al. Nano letters, **19**(4), 2516-2523 (2019).

[2] J. Comtet et al. Nature nanotechnology, **15**(7), 598-604 (2020).

[3] J. Comtet et al. Science Advances, **7**(40), eabg8568 (2020).

[4] N. Ronceray et al. Nature Materials, 1-7. (2020).

# Présentations

25 janvier 2024



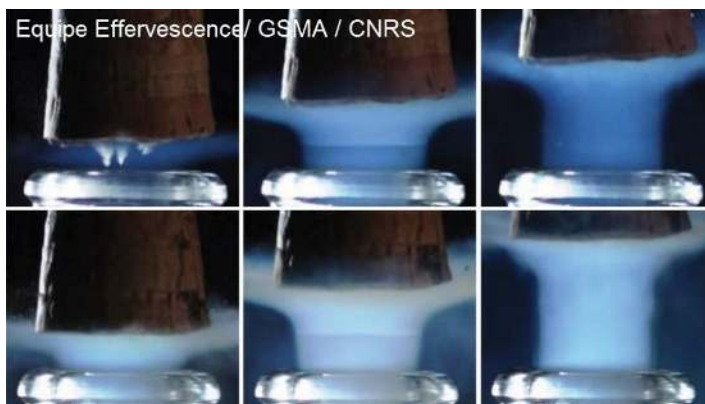
# Champagne! The science behind the bubble

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On average, nearly ten champagne corks pop every second across the globe! And this figure of course explodes on New Year's Eve. For several years now, champagne, and sparkling wines have experienced unprecedented growth. The waltz of bubbles in a flute is no stranger to this incredible craze. The effervescence that shakes your glass generates a host of phenomena of unsuspected complexity, which awakens all your senses. I offer you an overview of the physicochemical processes that accompany a champagne tasting, from uncorking the bottle to the bursting of a bubble, including the essential role of the glass in tasting. Deeply inscribed in the collective imagination, the champagne bubble becomes a pretext for a scientific stroll that will take you into the fascinating world of dissolved gases, phase changes and moving fluids. We will also show how this work on effervescence goes beyond the framework of a simple flute of champagne, to find analogies and possible applications in unexpected areas (on the surface of the oceans, and even to the confines of the solar system). You will discover the waltz of bubbles like you have never seen it before. Enjoy your trip to the heart of effervescence!



**Figure 1:** When the cork pops, under certain temperature and pressure conditions, the carbon dioxide under pressure in the bottleneck transforms into dry ice crystals (shown here by high-speed imaging). In the wake of the popping cork, we can even see a shock wave characteristic of supersonic flows.

## References

- [1] G. Liger-Belair, D. Cordier, R. Georges, Under-expanded supersonic CO<sub>2</sub> freezing jets during champagne cork popping, *Science Advances* 5, eaav5528 (2019).
- [2] G. Liger-Belair, *Un monde de bulles*, Ellipses, Paris (2020).
- [3] G. Liger-Belair and C. Cilindre, Recent progress in the analytical chemistry of champagne and sparkling wines, *Annual Review of Analytical Chemistry* 14, 21-46 (2021).

# Controlling magnetism by ionic liquid gating

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Magneto-ionics is a rapidly growing field in spintronics that offers great promise for the development of high-performance devices for information storage and processing. The ability to use electric fields to manipulate magnetic properties through ionic motion in a non-volatile way, presents exciting opportunities for the development of non-volatile and low-power memory devices. CoFeB and Pt/Co alloys are among the most technologically relevant materials for spintronics, therefore, the integration of magneto-ionics into Pt/Co and CoFeB-based devices can rapidly lead to new functionalities and enhanced performance.

Ionic liquid gating is a versatile technique used in various fields of materials science and condensed matter physics. It involves applying a voltage to an ionic liquid, which can be a room-temperature molten salt, causing ions to migrate to the interface of a material which, in turn, create a strong electric field. This highly efficient gating method does not need nanofabrication and can work over large areas, therefore, it is particularly useful in the study and manipulation of emergent properties in condensed matter systems.

In this talk, I'll give an overview on the effects and physico-chemical mechanisms at play in ionic liquid gating of CoFeB and Pt/Co alloys interfaced with a high ion mobility oxide [1-4]. In these materials, ionic gating induces the migration of oxygen-rich species within the stack, leading to large changes in the magnetic anisotropy and the Dzyaloshinskii-Moriya interaction in the magnetic layers but also important modifications in the crystalline structure of the oxide. I will show that the high degree of complexity of the magneto-ionic mechanisms and the strong influence of surface chemistry on the observed effects on the magnetic properties can be critical to define reversible and irreversible gating effects; which is of capital importance for the design of high performing and reliable spintronics devices relying on magneto-ionic gating.

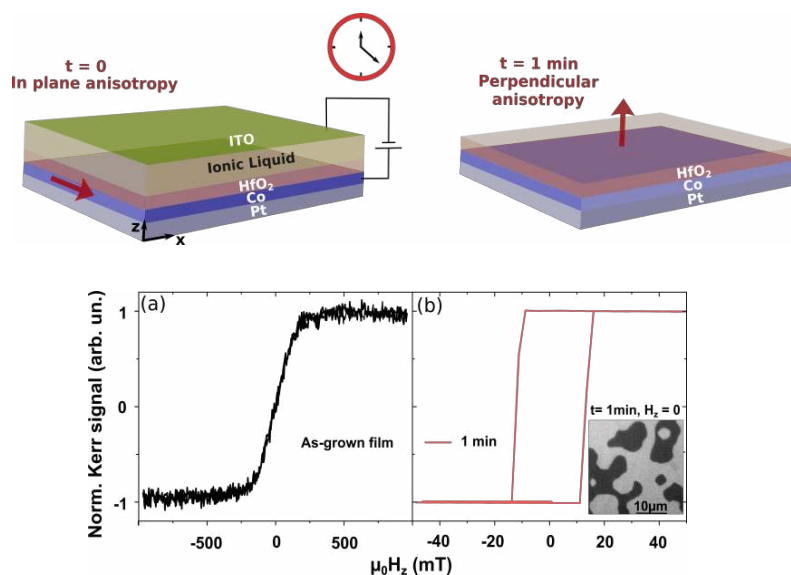


Fig.1. Ionic liquid gating configuration and magneto-ionic effects in a Pt/Co/HfO<sub>2</sub> system.

- [1] T. Bhatnagar-Schöffmann, et al.. Appl. Phys. Lett. 122, 042402 (2023).
- [2] R. Pachat et al., Adv. Mater. Interfaces, 2200690 (2022).
- [3] R. Pachat, et al.. Phys. Rev. Appl. 15, 064055 (2021).
- [4] L. Herrera Diez et al., Phys. Rev. Appl. 12, 034005 (2019).

# Chiralité magnétique aux interfaces : l'interaction de Dzyaloshinskii-Moriya

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L'interaction de Dzyaloshinskii-Moriya, un terme d'échange antisymétrique qui fait intervenir le produit vectoriel de deux spins voisins, a été introduite pour expliquer le moment ferromagnétique faible observé dans certains composés antiferromagnétiques, comme l'hématite  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub>. Ce terme, pour être non nul, impose que la symétrie d'inversion soit brisée. Dès l'origine, cette interaction a été reliée au couplage spin-orbite [1,2].

Albert Fert a fait remarquer dès 1990 que, une interface brisant la symétrie d'inversion, elle pouvait être le siège d'une telle interaction [3]. Mais ceci est resté théorique jusqu'à ce que les images de microscope à effet tunnel polarisé en spin révèlent des textures magnétiques chirales, dans les anti- comme les ferromagnétiques [4-6]. Il a fallu attendre quelques années de plus pour qu'on réalise la généralité de cette interaction, le système prototype étant une couche de quelques plans atomiques de cobalt déposée sur du platine texturé (111). Depuis, un grand nombre d'interfaces et d'architectures d'échantillons ont été testées, les mécanismes donnant lieu à cette interaction Dzyaloshinskii-Moriya d'interface ont été explorés par calculs de structure électronique, et aussi de nombreuses conséquences de cette interaction ont été découvertes, allant jusqu'à des idées d'applications. Une structure emblématique favorisée par cette interaction est le skyrmion magnétique.

Au cours de cet exposé on présentera ces différents aspects afin de faire le point sur l'état actuel des connaissances sur cette interaction.

[1] I.E. Dzyaloshinskii, Thermodynamic theory of « weak » ferromagnetism in antiferromagnetic substances, *Sov. Phys. JETP* **5**, 1259-1272 (1957).

[2] T. Moriya, New mechanism of anisotropic superexchange interaction, *Phys. Rev. Lett.* **4**, 228-230 (1960); Anisotropic superexchange interaction and weak ferromagnetism, *Phys. Rev.* **120**, 91-98 (1960).

[3] A. Fert, Magnetic and transport properties of metallic multilayers, *Mater. Sci. Forum*, **59-60**, 439-480 (1990).

[4] M. Bode, M. Heide, K. von Bergmann, P. Ferriani, S. Heinze, G. Bihlmayer, A. Kubetzka, O. Pietzsch, S. Blügel, R. Wiesendanger, Chiral magnetic order at surfaces driven by inversion asymmetry, *Nature* **447**, 190-193 (2007).

[5] P. Ferriani, K. von Bergmann, E. Y. Vedmedenko, S. Heinze, M. Bode, M. Heide, G. Bihlmayer, S. Blügel, R. Wiesendanger, Atomic-scale spin spiral with a unique rotational sense: Mn monolayer on W(001), *Phys. Rev. Lett.* **101**, 027201 (2008).

[6] S. Meckler, N. Mikuszeit, A. Pressler, E.Y. Vedmedenko, O. Pietzsch, R. Wiesendanger, Real-space observation of a right-rotating inhomogeneous cycloidal spin spiral by spin-polarized scanning tunneling microscopy in a triple axes vector magnet, *Phys. Rev. Lett.* **103**, 157201 (2009).

## From quantum dot to infrared imaging

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The Chemistry Nobel Prize this year celebrated the breakthrough of quantum dots, making it essential to highlight the practical achievements that led to this recognition. Quantum dots are semiconductor nanoparticles known for their size-tunable optical properties. In the late 1980s and early 1990s, their development marked a significant milestone, eliminating the constraints of metallurgy necessary for alloy production and overcoming epitaxy challenges posed by thin film growth. This innovation enabled the mass production of nanoparticles with atomic-like spectra. After nearly three decades of research, quantum dots found applications as biolabels, single photon sources, and solar cells. However, it was their use as phosphors in displays that catapulted them into the mass market. In this application, quantum dots function as optical downconverters, though challenges related to the electrical assessment of their optical features were often overlooked. Beyond light emission, quantum dots have immense potential as a disruptive technology for infrared sensing, a spectral range limited to a few semiconductors.

In my presentation, I will delve into a decade of advancements in infrared sensing using colloidal quantum dots. I will commence with the materials, tracing the evolution from the initial synthesis with mid-infrared absorption to the current high-performance materials [1]. Subsequently, I will discuss device development, emphasizing the field's complexity due to the introduction of light trapping strategies [2], increased pixel numbers [3-5], and meticulous control of carrier density to design phototransistors and photodiodes. I will showcase recent achievements in imaging, emphasizing how systematic measurements of electronic structure and precise determination of complex optical indices have been instrumental in these advancements.

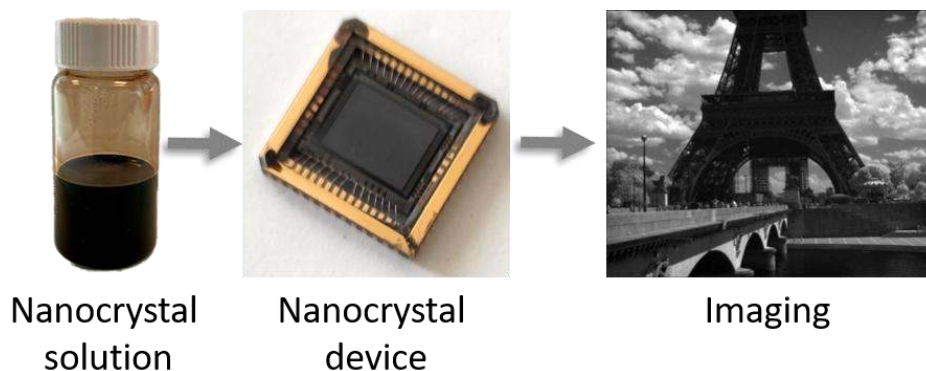


Fig.1 from quantum dot solution to infrared camera : a journey into colloidal optoelectronic

[1] C. Gréboval *et al.* *Chem. Rev.* 121, 3627 (2021)

[2] T.H. Dang *et al.*, *Nano Lett* 23, 8539 (2023)

[3] C. Gréboval *et al.*, *Nanoscale* 14, 9359 (2022)

[4] R. Alchaar *et al.*, *Appl Phys Lett* 123, 051108 (2023)

[5] Khalili, A. *et al.* *ACS Appl. Electron. Mater.* 5, 4377-4384 (2023)



## Building and characterizing artificial III-V lattices for quantum simulations

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The propagation of waves interacting with a periodical potential landscape leads to the formation of energy bands for wavelengths on the order of the lattice constant. By imposing a symmetry to the landscape, the band structure can be further tailored to create distinct energy-momentum dispersions, including conical intersections and nondispersive bands. Popular landscapes are the Su-Schrieffer-Heeger (SSH) chain in one dimension (1D) and the honeycomb, Dice, Lieb or Kagome lattices in two dimensions (2D). They have been experimentally tested for ultracold Bose gas, polaritons and photons and provide versatile platforms to emulate 1D and 2D Hamiltonians. For electrons, with de Broglie wavelengths in the nanometer scale or below, unique band structures shaped by the symmetry of the lattice are naturally found in graphene or have been designed with the manipulation of atoms or molecules on a metal surface. Transposing this approach to semiconductor heterostructures, in which the Fermi level, the carrier density and the lattice constant can be easily tuned, is particularly attractive as it would open new research fields in which geometric lattice concepts can be combined with spin-orbit coupling or with electronic or magnetic interactions for the study of new electronic phases. Here, I will explain how 2D and 1D lattices can be designed starting either from a semiconductor quantum well which is nanoperforated into a honeycomb lattice with lattice constant around 20 nm, or, using selective area epitaxy to produce complex nanowire geometries. I will consider the case of  $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}/\text{InP}$  and  $\text{InAs}/\text{InP}$  heterostructures. An essential point is that despite the multi-step process of nanopatterning, the semiconductor surfaces can be kept clean and atomically reconstructed, enabling the study of the subsurface electronic properties of the different structures with single and multiple-tip scanning tunneling microscopy. In particular, I will focus on the creation of 10 meV-wide dispersive bands and robust flat bands in the honeycomb lattice, the determination of the band offset at buried interfaces and the existence of ballistic charge transport.

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## Light experiments with infinite-layer nickelates

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The recent discovery of superconductivity in hole-doped Ni-based compounds [1] is shedding new light on the so-long-sought path towards the understanding of the high-temperature superconductivity. Nowadays, most of the ongoing research in infinite-layer nickelates is devoted at grasping differences and similarities with respect to cuprates, with which nickelates share square-planar structure and 3d-electron count. This recent discovery has re-vitalized the quest of new high-T<sub>c</sub> materials with unusual Ni<sup>1+</sup> and square-planar coordination, as initially suggested by a seminal theoretical work [2]. Soon after the first report, La- and Pr-based infinite-layer nickelates [3,4], and reduced square-planar Ruddlesden-Popper Nd<sub>6</sub>Ni<sub>5</sub>O<sub>8</sub> [5] thin films have also shown a zero-resistance state, assessing the importance of nickelates as a material platform to engineer novel superconductors.

In this talk, I will review our efforts to stabilize the infinite-layer phase going through some of the most important results obtained by studying the electronic properties of Nd<sub>1-x</sub>Sr<sub>x</sub>NiO<sub>2</sub> thin films [6,7] via means of various techniques. In particular, I will present scanning transmission electron microscopy measurements undertaken on uncapped NdNiO<sub>2</sub> thin films in collaboration with LPS lab in Orsay, that seem to solve the discrepancy of the charge order phenomenology [7-9], and reasonably associate the resonant signal originally attributed to a charge order of electronic nature, to an undesired surface-related structural reconstruction where stripes emerge from partially occupied apical oxygens [10]. Those stripes have been also independently reported on differently prepared samples, and associated indeed to a partially reduced infinite-layer phase [11]. I will end by introducing our latest results obtained in collaboration with UMPy lab in Palaiseau on (static) photo-stimulated experiments carried out by illuminating in the UV range SrTiO<sub>3</sub>-capped Nd<sub>0.95</sub>Sr<sub>0.05</sub>NiO<sub>2</sub> thin films grown onto different substrates. The observed large downturn of the sheet resistance for SrTiO<sub>3</sub>-grown samples will be discussed mainly in terms of a combination of strain and interfacial properties, while ruling out other possible effects ascribable to the photocarrier doping of the SrTiO<sub>3</sub> substrate itself.

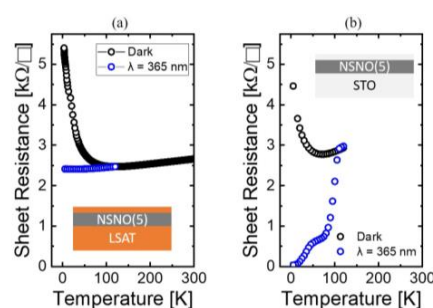


Fig.1 Transport properties of Nd<sub>0.95</sub>Sr<sub>0.05</sub>NiO<sub>2</sub>-NSNO(5) thin films for (a) LSAT and (b) STO grown samples in both dark (black) and UV-illumination (blue). Resistivity measurements acquired in van der Pauw configuration.

UMPhy lab in Palaiseau on (static) photo-stimulated experiments carried out by illuminating in the UV range SrTiO<sub>3</sub>-capped Nd<sub>0.95</sub>Sr<sub>0.05</sub>NiO<sub>2</sub> thin films grown onto different substrates. The observed large downturn of the sheet resistance for SrTiO<sub>3</sub>-grown samples will be discussed mainly in terms of a combination of strain and interfacial properties, while ruling out other possible effects ascribable to the photocarrier doping of the SrTiO<sub>3</sub> substrate itself.

- [1] Li, D. *et al.* Superconductivity in an infinite-layer nickelate. *Nature* **572**, 624–627 (2019).
- [2] Rice, T. M., M., A. V. & D., B. Electronic structure of possible nickelate analogs to the cuprates. *Phys. Rev. B - Condens. Matter Mater. Phys.* **59**, 7901–7906 (1999).
- [3] Osada, M., Yang Wang, B., Lee, K., Li, D. & Hwang, H. Y. *Phase Diagram of Infinite Layer Praseodymium Nickelate Pr<sub>1-x</sub>Sr<sub>x</sub>NiO<sub>2</sub> Thin Films*.
- [4] Osada, M. *et al.* Nickelate superconductivity without Rare-Earth Magnetism: (La,Sr)NiO<sub>2</sub>. *Adv. Mater.* **33**, 2104083 (2021).
- [5] Pan, G. A. *et al.* Superconductivity in a quintuple-layer square-planar nickelate. *Nat. Mater.* **21**, 160–164 (2022).
- [6] Krieger, G. *et al.* Synthesis of infinite-layer nickelates and influence of the capping-layer on magnetotransport. *J. Phys. D. Appl. Phys.* (2022).
- [7] Krieger, G. *et al.* Charge and Spin Order Dichotomy in NdNiO<sub>2</sub> Driven by the Capping Layer. *Phys. Rev. Lett.* **129**, 27002 (2022).
- [8] Tam, C. C. *et al.* Charge density waves in infinite-layer NdNiO<sub>2</sub> nickelates. *Nat. Mater.* **21**, 1116–1120 (2022).
- [9] Rossi, M. *et al.* A broken translational symmetry state in an infinite-layer nickelate. *Nat. Phys.* **18**, 869–873 (2022).
- [10] Raji, A. *et al.* Charge Distribution across Capped and Uncapped Infinite-Layer Neodymium Nickelate Thin Films. *Small n/a*, 2304872.
- [11] Parzyck, C. T. *et al.* Absence of Charge Density Wave Order in the Infinite Layer Nickelates. arXiv 2307.06486 (2023).

## Light on ferroelectric materials: epitaxial thin films and microdevices

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Ferroelectric materials are known to exhibit a reversible spontaneous electric polarization whose magnitude and sign can be precisely tuned, in particular by electric field. What makes ferroelectrics very interesting, by offering rich physics and a high potential for applications, is the coupling between their electric polarization and other properties. The coupling between electric polarization and mechanical deformation leads, for instance, to remarkable piezoelectric response with numerous applications in microelectromechanical systems (MEMS) - actuators and sensors. Their interaction with light has shown above bandgap photovoltages, induced by a particular polarization-related charge-separation mechanism in ferroelectrics, the so-called bulk photovoltaic effect. In addition, the complex interplay between light, ferroelectric polarization, and deformation induces photostriction – a mechanism of non-thermal deformation under illumination – which is usually described in a ferroelectric as a combination of photovoltaic and piezoelectric effects. Photo-induced effects in ferroelectrics offer thus a wide field of possible investigations into interesting physics and exciting new applications [1, 2], with the potential for remote (optical) control.

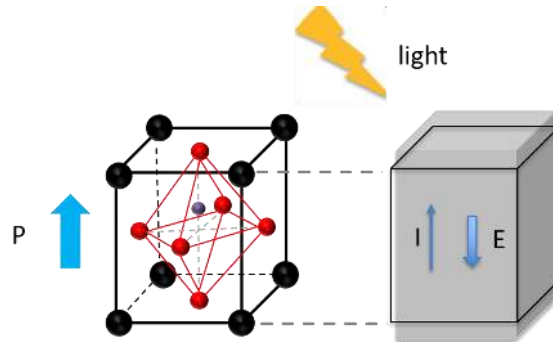


Fig.1. Sketch of photo-induced effects in a ferroelectric material. (Left) Crystalline unit cell with ferroelectric polarization  $P$ . (Right) Generation under light of current  $I$ /electric field  $E$  (photovoltaic effect) and deformation (photostriction).

In this talk, I will present studies on the control of photovoltaic effect and photostrictive response by tuning the ferroelectric polarization in the prototypical  $\text{Pb}(\text{Zr},\text{Ti})\text{O}_3$  ferroelectric material, epitaxially grown in thin films and integrated into microdevices [3, 4]. This tunability has been used to develop innovative optically controlled microelectronic devices. First, a non-destructive optical reading of the polarization state will be reported in non-volatile multistate ferroelectric memories [5], offering great promises for increased data storage density and lower power operation. Second, a non-thermal optical control of deformation will be demonstrated, providing light-induced expansion or contraction, exploited in microcapacitors and MEMS. These results have important implications for the light-mediated engineering of materials and devices functionalities.

- [1] B. Kundys, *Appl. Phys. Rev.* **2**, 011301 (2015)
- [2] C. Paillard, et al., *Adv. Mater.* **28**, 5153–68 (2016)
- [3] K. Rani, et al., *J. Phys: Condens. Matter* **34**, 104003 (2022)
- [4] S. Matzen, et al., *Adv. Elec. Mater.* **5**, 1800709 (2019)
- [5] A. Zing, et al., *Appl. Phys. Lett.* **121**, 232904 (2022)

## Coupling of metal-insulator transitions in nickelate based superlattices

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Perovskite nickelates ( $\text{RENiO}_3$ , RE=Rare Earth, RE $\neq$ La) are fascinating materials, well-known for their metal to insulator transition (MIT) and unique antiferromagnetic ground state [1-3]. In this presentation, I will discuss the phase diagram of the system and the physics of the MIT before focusing first on  $\text{NdNiO}_3/\text{SmNiO}_3$  superlattices that display, depending on the thickness of the individual layers, a single or double MIT. The electronic state of the materials was revealed at the unit cell scale using Scanning Transmission Electron Microscopy [4]. The critical wavelength  $\Lambda_c$  below which a single MIT is observed is 16 unit cells. This model system allows the origin of the coupling at such oxide interfaces to be studied. The key finding is that the critical length scale is not set by the length scale of the propagation of structural motifs (Ni-O-Ni bond angles) across the interface between the two materials, which ab-initio calculations and STEM analyses suggest is minimal, but rather by the balance between the energy cost of having metallic-insulator – phase boundaries and the energy gain of the bulk phases [5]. I will then show how the insertion of ultrathin layers (1-4 unit cells) of insulating  $\text{LaAlO}_3$  allows a complete decoupling of the MIT's [6]. Finally, I will describe very recent experiments where we use this phase boundary cost to turn a metal into an insulator.

[1] M.L. Medarde, Journal of Physics Condensed Matter 9, 1679 (1997)

[2] G. Catalan, Phase Transitions 81, 729 (2008)

[3] S. Catalano et al., Reports on Progress in Physics 81, 046501 (2018)

[4] B. Mundet et al. Nano Letters 21, 6, 2436 (2021)

[5] C. Dominguez et al. Nature Materials, 19, 1182 (2020)

[6] L. Varbaro et al. Advanced Electronic Materials 2201291 (2023)

# Présentations

26 janvier 2024



## Using magnetism to act on living cells

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The mechanical vibration of magnetic particles under low frequency magnetic field allows applying mechanical stress at the cell level. The magnetic particles are designed to have superparamagnetic-like properties to avoid agglomeration [1] and sufficiently large volume to exert forces in the pN range to produce significant mechanobiological reactions on cells. This mechanical stress, tunable through the characteristics of the applied magnetic field, induces a large variety of physiological reactions depending on the nature of the cells and on the intensity of the magneto-mechanical stimulation. The mechanical stress has a strong influence on the cells cytoskeleton which triggers a variety of signalling pathways.

Using U87 glioma brain cancer cells, we observed that a weak stimulation induces already a disorganization of the cell cytoskeleton resulting in a cell contraction, a loss of motility and a stop of the mitosis. A stronger stimulation can induce the apoptosis (spontaneous death) of the cells [2-4]. Thus, a stimulation with a moderate alternating field of 20mT at 20Hz for 30minutes induces the death of 80% of the cancer cells (Fig.1). Remarkably, the still alive cells do not proliferate anymore during several days. The magneto-mechanical treatment can be repeated until the cancer cells are fully destroyed. This approach can lead to a new approach towards cancer treatment, used alone or in conjunction with chemotherapy.

Studies on cancer cells were conducted *in-vitro* as well as *in-vivo* revealing quite different results for a variety of reasons. Ongoing studies are carried out on spheroids of cells embedded in 3D gels which represent *in-vitro* models much closer to *in-vivo* situations.

Experiments were also conducted on pancreatic cells [5]. We demonstrated that the magnetically induced mechanical stimulation of pancreatic cells allows enhancing insulin secretion. This observation can also open a new route towards innovative diabetes 2 treatments [5] whereby the insulin level of a diabetic patient would be increased not by injection of insulin with a syringe but by an external magnetic field with magnetic particles being permanently dispersed in the pancreas.

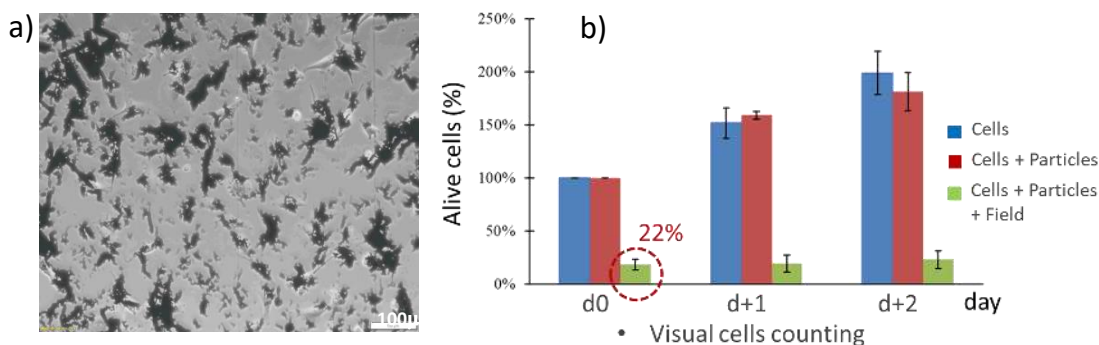


Fig.1: a) Glioma cancer cells incubated with NiFe vortex microdisks. Interestingly, the cells catch all magnetic particles even without functionalization. b) In vitro testing of magneto-mechanical stimulation of glioma cells. Blue and red bars correspond to controls (cells without particles and cells with particles but no oscillating field), green bar: Cells with particles submitted to oscillating field (20mT, 20Hz). ~80% of the cancer cells die after treatment. Interestingly, the still alive ones do not proliferate during several days.

[1] H.Joisten et al, Appl. Phys. Lett. 97, 253112 (2010)

[2] S.Leulmi et al, Nanoscale, 7 (2015) 15904

[3] C.Naud et al, Nanoscale Adv., 2 (2020) 3632

[4] C. Thébault, Nanoscale Advances, 3, 6213 (2021)

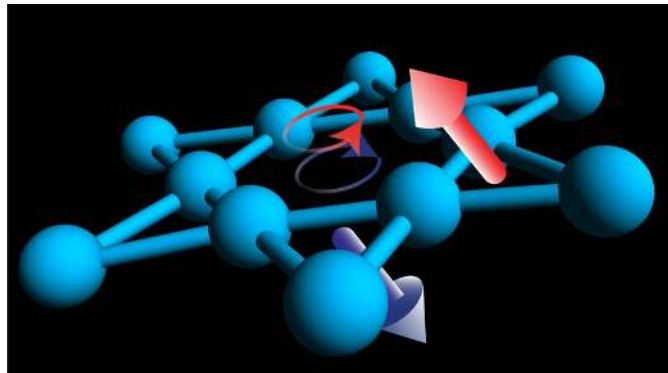
[5] S.Ponomareva et al, Nanoscale, 14 (2022) 13274

## The art of seeing electrons and playing with their spins

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After the rise of graphene in 2010, the discovery of exotic topological phases has become the hinge of a revolutionary concept: The currents can be generated by using the electron spins. Such currents, the so-called spin-currents, offer innumerable advantages compared to the classical ones: They are protected against disorder and can be transported without backscattering of carriers. This minimizes the power that allows the electronic devices to work, enabling technology to operate at a considerably lower switching energy. In this context, investigating and manipulating the spins of the electrons constitutes a unique opportunity to stabilize exotic phases of quantum matter which are currently beyond reach and to understand the ones which are still significantly unexplored.

Here, I will present a new methodology to investigate the spin-driven properties of Kagomé systems I will show how to move beyond the current state of the art and present the ability to measure the topological invariants directly, exemplified by the Berry phase.



### References

Di Sante,..., Mazzola, Nature Physics 19, 1135-1142, 2023

## L'eau comme source de charge ou comme ligand aux interfaces liquide-solide

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La dynamique des fluides à l'échelle nanométrique, ou nanofluidique, est un domaine de recherche émergent où le continuum de l'hydrodynamique rencontre la nature atomique de la surface de confinement.

Lorsque la surface est un matériau 2D comme le graphène, la haute performance des écoulements d'eau à l'échelle nanométrique a longtemps défié une compréhension rationnelle. Étant donné que certains matériaux 2D peuvent former des membranes à grande échelle, la rationalisation de ces performances est indispensable pour le développement de nouvelles membranes biosourcées.

Partant des mesures nanofluidiques qui démontrent que des matériaux 2D idéaux (comme le graphène et son analogue structural hBN) acquièrent d'importantes charges négatives de surface lorsqu'ils sont immergés dans des solutions aqueuses, nous rationaliserons l'origine de cette charge extrinsèque de surface à l'aide de simulations ab initio MD (AIMD) [1].

Puis nous expliquerons pourquoi l'eau moléculaire réagit sur des matériaux 2D 'défectueux' tels que l'oxyde de graphène [2] et un défaut de type catalyseur à atome unique Fe-N<sub>4</sub> dans le graphène [3], en soulignant la nécessité d'inclure l'eau solvant de manière explicite dans les simulations quantiques. Comme résultat clé, de telles réactions chimiques interfaciales alimentent spontanément l'eau liquide en protons, indispensables pour l'électrocatalyse.

[1] B. Grosjean, M.-L. Bocquet, R. Vuilleumier, Nat. Comm. **10**, 1656 (2019).

[2] F. Mouhat, F.X. Coudert, M.-L. Bocquet, Nat.Comm. **11**, 1566 (2020).

[3] L. Scalfi, M. R. Becker, R. R. Netz, M.-L. Bocquet, Commun.Chem. in press (2023).

## Modelling electronic transport in 2D materials

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2D materials have shown fascinating fundamental physics as well as exciting technological prospects, from transistors to integrated optoelectronics. Many applications rely on the ability of the 2D material to conduct electrons efficiently. At room temperature, this is mostly limited by the scattering of electrons by phonons. A clear understanding of the electronic transport mechanisms, along with predictive ab initio simulations [1], are then key to design performant and energy-efficient devices.

In this framework, 2D materials present 3 major peculiarities: their reduced dimensionality, the ability to tailor their properties by combining different layers in a van der Waals heterostructure, and the ubiquitous usage of electrostatic doping. The latter refers to the field-effect transistor configuration, in which a gate is used to induce charges in the 2D material and change its Fermi level.

We will explore the consequences of those 3 peculiarities on electron-phonon interactions and the scattering mechanisms [2-3]. We will see how to compute the macroscopic quantities characterizing the transport of electrons through the material [4] and discuss the performances of various layers [5] taken from a database of exfoliable 2D materials build with high-throughput ab initio workflows [6].

[1] S. Poncé, W. Li, S. Reichardt, and F. Giustino, *First-Principles Calculations of Charge Carrier Mobility and Conductivity in Bulk Semiconductors and Two-Dimensional Materials*, Reports on Progress in Physics **83**, 036501 (2020).

[2] T. Sohier, M. Gibertini, and M. J. Verstraete, *Remote Free-Carrier Screening to Boost the Mobility of Fröhlich-Limited Two-Dimensional Semiconductors*, Phys. Rev. Materials **5**, 024004 (2021).

[3] T. Sohier, P. M. M. C. De Melo, Z. Zanolli, and M. J. Verstraete, *The Impact of Valley Profile on the Mobility and Kerr Rotation of Transition Metal Dichalcogenides*, 2D Mater. **10**, 025006 (2023).

[4] T. Sohier, D. Campi, N. Marzari, and M. Gibertini, *Mobility of 2D Materials from First Principles in an Accurate and Automated Framework*, Physical Review Materials **2**, 114010 (2018).

[5] T. Sohier, M. Gibertini, and N. Marzari, *Profiling Novel High-Conductivity 2D Semiconductors*, 2D Materials **8** 015025 (2020).

[6] Materials Cloud two-dimensional crystals database, <https://www.materialscloud.org/discover/mc2d>

# Posters

25 janvier 2024



# Matériaux 2D

## Molecular adsorption on Dumbbell Silicene

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Following graphene discovery, 2D materials attracted rising attention due to their remarkable properties. Among them, silicene has been particularly studied as Si is essential in semi-conductor industry. Silicene presents an electronic structure very similar to the one of graphene [1], but is more sensitive to chemical environment. The possibility of tuning the electronic properties of silicene by molecular adsorption associated with the 2D geometry makes it a promising candidate for highly sensitive molecular sensors.

We have recently proven the existence of Dumbbell Silicene (DBSi) obtained by thermal evaporation of Si onto Ag(110) at 200°C [2]. It shows a low density of adatoms, on top of Si atoms of the silicene layer (Fig. 1b), forming DB units. Adsorption of molecules onto these sites is expected to open a small gap in the electronic structure, while preserving the overall silicene band structure [3].

Using operando STM, we have followed the evolution of DBSi upon exposure to ammonia (NH<sub>3</sub>) and have noticed that depending on the temperature at which the experiment was carried out, the system behaved differently. At room temperature (RT), if some molecules adsorb on top of DBs, other molecules are found to adsorb on the DB free regions silicene or on defects of the surface. Adatoms on DBSi are not strong preferential adsorption sites, contrary to what we observed for the SiC(0001)-(3x3) reconstruction. Its surface is very similar to the one we study: having a Si-rich termination of SiC and possessing a small density of adatoms as well.

On the other hand, at low temperature, we can spot a clear preference of adsorption of ammonia on top of DB sites as sought for the goal exposed above. Moreover, as expected by cooling down the sample, the physisorption is favoured which lead to an increase of chemisorbed molecules too, that will stay fixed on top of the DBs once the sample is back to room temperature (Fig. 1c). The chemisorption is here in a competition with the desorption and happens only if the energy barrier is overcome. A dissociative adsorption is expected here via N-H bond cleavage, as it is the case on other silicon crystal surfaces [4]. Furthermore, the quantity of the adsorbed molecules at 123K is similar to the one at RT with an exposure to NH<sub>3</sub> hundreds of times more important. Therefore, at low temperature, for ammonia the DB sites are by far more reactive than the rest of the silicene layer.

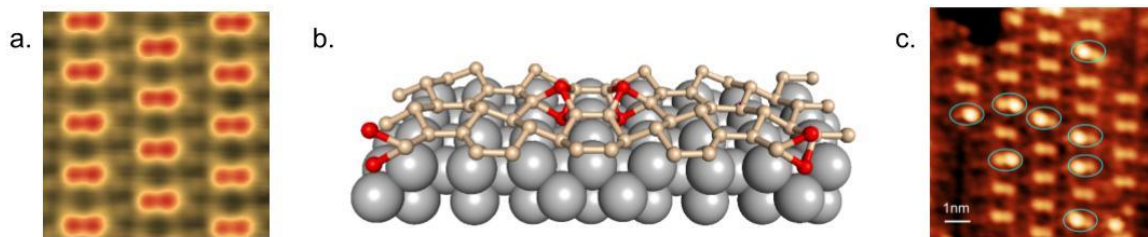


Fig. 1. a) STM image of the periodic DBSi mono-layer (5x5 nm<sup>2</sup>) on Ag(110). b) schematic of silver substrate (gray) with the silicene layer above and the DBSi (highlighted in red). c) STM images of NH<sub>3</sub> adsorbed on Dumbbell Silicene at 123K (Height of the DBs ≈ 85pm; Height of the NH<sub>3</sub> adsorbed on DB ≈ 50pm)

[1] Cahangirov, S. et al., Phys. Rev. Lett. **102**, 236804 (2009)

[2] Leoni, T. et al., J. Phys. Chem. C, **125**, 17906–17917 (2021)

[3] V. O. Özçelik et S. Ciraci, J. Phys. Chem. C, **117**, 26305-26315 (2013)

[4] Mathieu, C. et al. J. Phys. Chem. C **113**, 11336–11345 (2009)

## From surface alloys to "germanene": Ge/Ag(111) growth

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Two-dimensional (2D) honeycomb lattices beyond graphene, such as germanene, appear very promising due to their outstanding electronic properties, such as quantum spin hall effect. While there have been many claims of germanene growth, experimental evidence for a honeycomb structure has only been obtained indirectly, from STM observations or electronic properties measurements.

Among all the potential substrates for germanene growth, Ag(111) which is known to be well suited for the growth of silicene, is undoubtedly the most discussed one today. On this substrate, the structures observed have been either described as honeycomb germanene or surface alloys. Using scanning tunneling microscopy (STM), surface X-ray diffraction and density functional theory, we have studied the structure and energetics of germanium layers on Ag(111) in the 400K-450K temperature range [1-3]. We show that upon increasing coverage, a series of alloyed phases forms. Two of these phases correspond to highly ordered reconstructions for which we determined precisely the atomic structure. The first one is a  $c(31\times\sqrt{3})$  reconstruction corresponding to a  $\text{Ag}_2\text{Ge}$  surface alloy with an atomic density 6.45% higher than the Ag(111) atomic density. It is formed by stripes associated with a face-centered cubic top-layer alignment, alternating with stripes associated with a hexagonal close-packed top-layer alignment, in great analogy with the  $(22\times\sqrt{3})$  Au(111) reconstruction [2]. The second one is a  $(\sqrt{109}\times\sqrt{109})$  reconstruction, composed of a periodic arrangement of Ge pentagons, hexagons and heptagons with a small concentration of Ag atoms [3]. Our result opens new perspectives related to the understanding of the complex structures observed after growth of Ge or Si on metal surfaces.

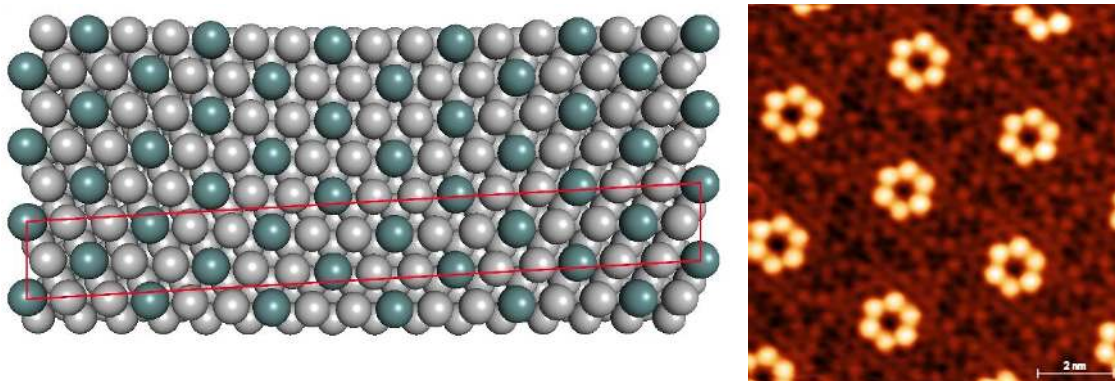


Fig. a) Top view of the atomic structure of the  $c(31\times\sqrt{3})$  reconstruction.  
b) STM image ( $8.5\times 8.5\text{ nm}^2$ ) of the  $(\sqrt{109}\times\sqrt{109})$  reconstruction.

[1] K. Zhang, R. Bernard, Y. Borensztein, H. Cruguel, G. Prévot, Phys. Rev. B 102 (2020) 125418

[2] K. Zhang, *et al.*, Phys. Rev. B 104 (2021) 155403

[3] K. Zhang *et al.*, ACS Nano, 1 (2023) 15687

# Graphène à bandes plates créé par des déformations périodiques

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Le nombre d'études des propriétés électroniques de matériaux 2D ou de types Van der Waals n'a cessé d'augmenter depuis ces dernières années, notamment pour les études sur le graphène et de ses propriétés électroniques intéressantes. Par exemple, il est possible de faire émerger des phases électroniques corrélées comme de la supraconductivité ou des états d'isolants corrélés dans les moirés de graphène [1]. En effet, selon l'angle entre deux couches de graphène, il existe des conditions où la vitesse de Fermi s'annule pour certains angles, dits 'magiques' [2]. Cet aplatissement des bandes permet l'accès à un régime où l'énergie de Coulomb domine l'énergie cinétique effective des électrons ce qui donne naissance aux nouvelles phases observées. L'inconvénient des moirés de graphène et la difficulté de fabrication des échantillons d'une part et la faible stabilité mécanique de la structure ce qui peut limiter les effets des corrélations électroniques recherchés expérimentalement [3].

Une autre manière de valider ces critères sans avoir les défauts des moirés serait de déformer périodiquement une feuille de graphène. En effet, les déformations engendrent des pseudo-champ magnétiques (fig. 1. a) donnant lieu à des pseudo-niveaux de Landau et donc une physique de bandes plates [4,5]. Nous présentons des calculs de structure de bande de graphène déformé périodiquement comme présenté figure (fig. 1. b). Ces calculs par un modèle de liaison forte ont pour but de déterminer l'influence de l'orientation relative de la déformation périodique et du réseau cristallin pour guider les études expérimentales à venir.

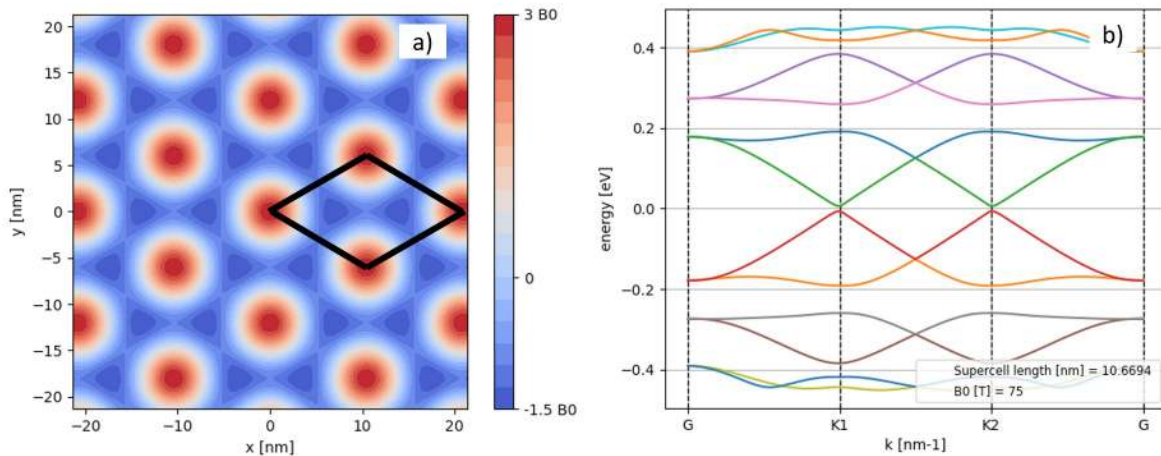


Fig.1. (a) Profil d'un pseudo-champ magnétique périodique sur graphène et le schéma de la supercellule de calcul en noir (b) Structure de bande pour un champ  $B_0$  de 75 T et pour une longueur de supercellule de 10.67 nm.

- [1] Cao, Y., Fatemi, V., Fang, S. et al. Nature 556, 43–50 (2018).
- [2] R. Bistritzer, A.H. MacDonald, PNAS, 108(30):12233 12237, 2011
- [3] F. Mesple, "Experimental study of heterostrain in moiré superlattices of graphene bilayers", 2022
- [4] J. Mao, S.P. Milovanović, M. Anđelković, et al. Nature 584, 215–220 (2020).
- [5] S. P. Milovanović, M. Anđelković, L. Covaci, and F. M. Peeters Phys. Rev. B 102, 245427, 2020

# Hétérostructures



## IrCo upstanding heterodimers on graphene: highly anisotropic magnetic moments protected from their environment?

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Quantum bits are extensively studied by their potential for quantum computing, communication and metrology but also because they are fascinating platforms to understand the behavior of quantum matter, in a controlled, designed-at-will, manner. The case of single magnetic molecules and **single magnetic atoms on surfaces** has been proved to be a rich playground to address the properties of both electronic and nuclear spins [1]. Understanding the quantum levels, how they are influenced by the local environment and the mechanisms leading to spin relaxation are key questions in this field. In particular, the research for stable magnetic moments with high magnetic anisotropies (MAE) and protected from the electronic and crystal environment is a very active quest [2], because it would lead to magnetic memories with huge density information.

Several theoretical studies have proposed transition metal dimers as being promising candidates to find long life-time magnetic moments with large MAE. First calculations focused on gas phase dimers [3], but progressively they moved to the on-surface case [4]. Here, we concentrate on the **3d-5d heterodimers on a graphene layer** [5]. The 3d elements (Fe or Co) are characterized by a large magnetic moment, while the 5d ones (Pt, Ir) have a large spin-orbit coupling. The combination of both ingredients is usually responsible for large MAE. Moreover, the graphene acts as a decoupling layer which isolates the magnetic moments from phonons and electrons of the surface (usually graphene is grown on metal substrates), thus improving the magnetic stability. Finally, it has been shown that some of these heterodimers, such as IrCo, are expected to be upstanding on a graphene layer (both for free-standing graphene and for Gr/Cu(111)). The upstanding geometry implies that the top atom (Ir in this case) is not influenced by the crystal field of the surface, i.e. the crystal field symmetry is an axial one ( $C_{\infty}$ ). The possible magnetization reversal paths due to tunneling are determined by the crystal field, the higher the symmetry the more the quantum levels are protected. All these characteristics together make **IrCo/Gr** an excellent candidate to study **magnetic stability of 3d-5d heterodimers**.

We will show the recent progress in the synthesis and experimental study of IrCo heterodimers developed in our team. At first, we will present some preliminary results showing the formation of IrCo heterodimers on a Gr/ Ir(111) surface. These samples are grown under ultra-high-vacuum and measured at low temperature (4K) using spin polarized scanning tunneling microscopy (SP-STM). We observed structural instability of the upstanding heterodimers, as well as complex magnetic switches suggesting the existence of several structural-magnetic configurations. Secondly, we will discuss the existence of IrCo heterodimers on a Gr/Cu(111) surface, whose properties have been theoretically studied [5]. Our first measurements suggest the formation of some upstanding heterodimers, which seem to be strongly perturbed by the STM tip and give large magnetic contrast when measured by SP-STM.

[1] S. Loth et al., *Science* **329**, 1628 (2010); Thiele et al., *Science* **344**, 1135 (2014)

[2] F. Donati et al., *Science* **352**, 318 (2016); R. Baltic et al., *Nanolett.* **16**, 7610 (2016); A. Singha et al., *Nat Commun* **12**, 4179 (2021)

[3] T. O. Strandberg et al., *Nat. Mater.* **3**, 648 (2007); L. Fernandez-Seivan et al., *PRL* **99**, 183401 (2007)

[4] H. Johll, et al., *PRB* **79**, 245416 (2009); Longo et al., *PRB* **81**, 115418 (2010); Srivastava et al., *PRB* **85** 165444, (2012)

[5] P. Blonski et al., *J. Phys. Cond. Matter* **26**, 146002 (2014); P. Blonski et al., *J. Phys. Cond. Matter* **26**, 256001 (2014)

## Towards the stabilization of infinite-layer nickelate freestanding films

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The recent discovery of superconductivity in hole-doped infinite-layer nickelate thin films has sparked renewed interest in the condensed matter community [1]. This is motivated by the possibility of adding another puzzle piece to the understanding of unconventional superconductivity, a phenomenon that has not yet been observed in infinite-layer polycrystalline samples [2]. In infinite-layer nickelate, the substrate induced strain is suspected to play a key role in stabilizing the phase of superconductivity. Inspired by recent advances in the epitaxial lift-off of oxide films, our idea to control the strain of those films is to free them from substrate-induced stresses. Freestanding films, as demonstrated for perovskite thin films, can exhibit a variety of functionalities [3].

In this context, here, we present our preliminary results on the use of epitaxial lift-off techniques to fabricate freestanding layers of nickelate films (Fig. 1) with the final goal to perform a topotactic reduction process. By using a pulsed laser deposition (PLD) technique and assisted by high-energy reflection electron diffraction (RHEED), we have epitaxially grown (Nd,Sr)NiO<sub>3</sub>-based heterostructures on a sacrificial layer of water-soluble (Ca,Sr)<sub>3</sub>Al<sub>2</sub>O<sub>6</sub> [4]. These sacrificial layers are particularly adapted to study the effect of the strain on the stabilization of the infinite-layer phase. By selecting an opportune Ca/Sr ratio, the sacrificial layer can be grown on various substrates, therefore, enhancing the integrity of the released layers and minimizing crack formation [5]. Here, we show that freestanding layers as large as 5x5 mm<sup>2</sup> can be fully transferred on PET or PDMS support. Structural analyses conducted via X-ray diffraction and atomic force microscopy confirm the preservation of the crystalline quality of the layers, close to that of the seed films.

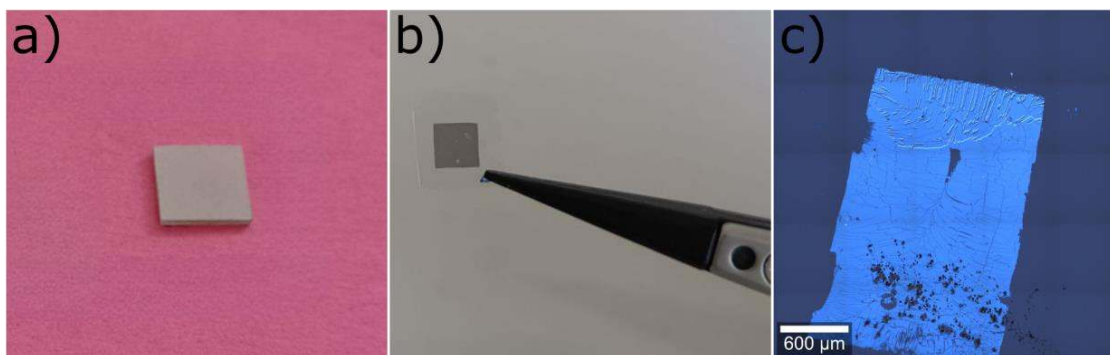


Fig.1. a-b) Photograph of nickelate heterostructure on SrTiO<sub>3</sub> substrate and polymer support respectively, c) Optical microscope image of a layer transferred to SiO<sub>2</sub> substrate.

[1] Li, D.; Lee, K.; Wang, B. Y.; Osada, M.; Crossley, S.; Lee, H. R.; Cui, Y.; Hikita, Y.; Hwang, H. Y. *Nature* 2019, 572, 624–627.

[2] Li, Q.; He, C.; Si, J.; Zhu, X.; Zhang, Y.; Wen, H.-H. *Commun. Mater.* 2020, 1, 16.

[3] Pesquera, D.; Fernandez, A.; Khestanova, E.; Martin, L. W. *Journal of Physics: Condensed Matter* 2022, 34, 383001.

[4] Lu, D.; Baek, D. J.; Hong, S. S.; Kourkoutis, L. F.; Hikita, Y.; Hwang, H. Y. *Nature materials* 2016, 15, 1255–1260.

[5] Prodjosantoso, A.; Kennedy, B. *Journal of Solid State Chemistry* 2002, 168, 229–236.

# Croissance, épitaxie

## Growth mode and equilibrium shapes of core(Fe)@shell(Au) nanoparticles as a function of the metals volume ratio

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The equilibrium shape of nanoparticles is investigated to elucidate the various core-shell morphologies observed in a bimetallic system associating two immiscible metals, iron and gold, that crystallize respectively in the bcc and fcc lattices. Fe@Au core@shell nanoparticles present a crystalline Fe core embedded in a polycrystalline Au shell, with core and shell morphologies both depending on the Au/Fe volume ratio [1]. A model [2] is proposed to calculate the energy of these nanoparticles as a function of the Fe volume, Au/Fe volume ratio, core shape and shell shape, using the DFT-computed energy densities [3] of the metal surfaces and of the two possible Au/Fe interfaces. Three driving forces leading to equilibrium shapes were identified: the strong adhesion of Au on Fe, the minimization of the Au/Fe interface energy that promotes one of the two possible interface types, and the Au surface energy minimization that promotes a 2D-3D Stranski-Krastanov like transition of the shell [2]. For low Au/Fe volume ratio, the wetting is the dominant driving force and leads to the same polyhedral shape for the core and the shell, with an octagonal section. For large Au/Fe ratio, the surface and interface energy minimizations can act independently to form an almost cube-shaped Fe core surrounded by six Au pyramids. The experimental nanoparticles shapes [1, 4] are well reproduced by the model, for both low and large Au/Fe volume ratios [2].

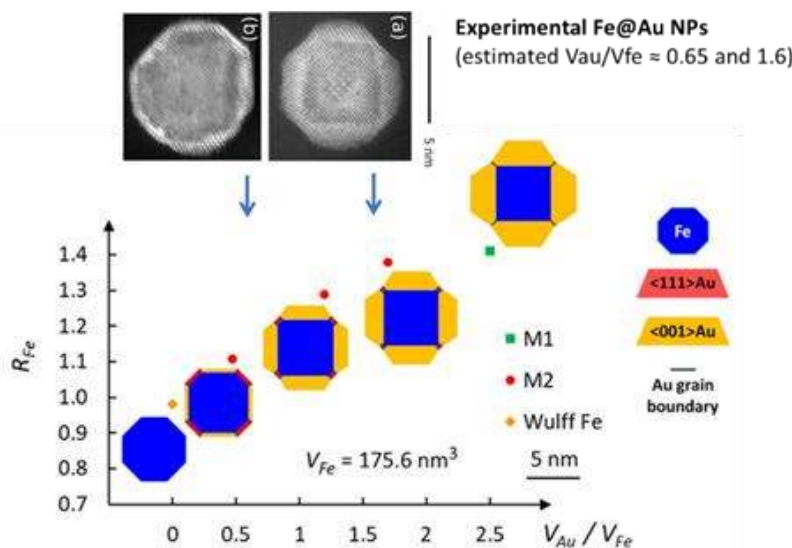


Fig.1 : Evolution of the equilibrium shape of Fe@Au nanoparticles, as a function of the Au/Fe volume ratio [2].

[1] P. Benzo, S. Combettes, B. Pecassou, N. Combe, M. Benoit, M. Respaud, and M. J. Casanove, *Phys. Rev. Mater.* 3, 096001 (2019)

[2] A. Ponchet, S. Combettes, P. Benzo, N. Tarrat, M.J. Casanove and M. Benoit, *J. Appl. Phys.* 128, 055307 (2020) [hal-02913274v2](https://arxiv.org/abs/2009.13274)

[3] S. Combettes, J. Lam, P. Benzo, A. Ponchet, M.-J. Casanove, F. Calvo and M. Benoit - *Nanoscale*, 12, 18079 (2020) [hal-02989677](https://arxiv.org/abs/2009.09677)

[4] S. Combettes, T. Hungria, S. Barre, B. Pecassou, R. Cours, M. Benoit, M.-J. Casanove, A. Ponchet, and P. Benzo - *Eur. Phys. J. Appl. Phys.* 97, 27 (2022) [hal-03685120](https://arxiv.org/abs/2203.03685)

# Ferroelectricity of GeTe thin films grown on miscut Si substrates

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Thermoelectric modules are solid-state energy converters that allow direct and reversible conversion of heat into electricity and are considered as a promising clean-energy technology [1]. The past decade has witnessed a sustained boom in new thermoelectric materials, among which GeTe has shown one of the highest performances [2]. So far, thermoelectrics have been optimized *via* the increase of electric conductivity and a decrease of thermal conductivity through defects to increase phonon scattering. We propose to enhance the thermoelectric properties of GeTe *via* the control of ferroelectricity. Indeed

ferroelectric materials such as GeTe bring an additional degree of freedom, the electric polarization. GeTe thin films contain different polarization states known as ferroelectric domains that are separated by narrow interfaces, called domain walls, where large structural distortions occur. These lattice distortions may couple to phonons and considerably reduce the thermal conductivity. In addition, polarization discontinuities may trap free charge carriers and enhance the electrical conductivity. Therefore we propose to engineer ferroelectricity at the nanoscale to drive the thermoelectric performances.

In order to tackle the ferroelectric properties of GeTe thin films we have used Transmission Electron Microscopy (TEM), Low Energy Electron Microscopy (LEEM) as well as *in situ* X-ray diffraction [3-5]. The GeTe thin films are grown by Molecular Beam Epitaxy (MBE) on nominal and miscut Si substrates. We highlight the role of the miscut angle on the growth and ferroelectric domains of GeTe thin films.

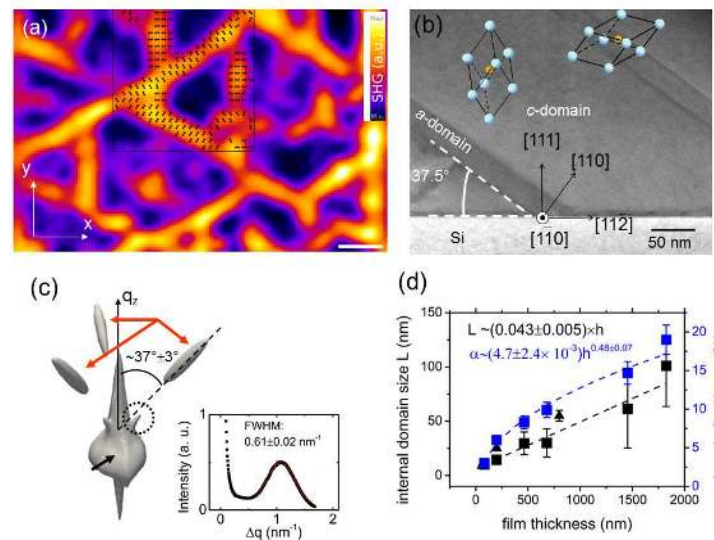


Figure: (a) Isotropic secondary harmonic generation (SHG) image revealing the domain structure of a 1825 nm-thick GeTe film. The black arrows indicate the local in-plane polarization orientation in the nanodomains. The a-domains contributions (yellow-orange) with in-plane polarization are superimposed to the background (dark-purple) signal exhibiting out-of-plane polarization (c-domains). Scale bar 5  $\mu\text{m}$ . (b) Cross-section TEM showing inclined a-domains inside the GeTe layer on Si(111). (c) 3D-reciprocal space map obtained by X-ray diffraction showing 4 Bragg peaks from c-domains (black arrow) and a-domains (red arrows). (d) a-domains size and volume fraction as function of GeTe film thickness.

[1] E. Ghafari *et al.*, Wiley-VCH Verlag, 173-182 (2018)

[2] M. Hong *et al.*, Adv. Mater. 31, 1807071 (2019)

[3] B. Croes *et al.*, Phys. Rev. Mat. 5 124415 (2021)

[4] B. Croes *et al.*, Phys. Rev. Mat. 6 064407 (2022)

[5] B. Croes *et al.*, Phys. Rev. Mat. 7 014409 (2023)



# Morphology and symmetry driven by lattice accommodation in polycrystalline bcc-fcc core-shell metallic nanoparticles

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Bcc-fcc multi-metallic nanoparticles (NPs) associating a single-crystal core (Fe, FeCo alloys...) with a polycrystalline noble metal shell (Au, AuAg alloys ...) are perfectly symmetrical [1, 2] or more irregular, even dramatically dissymmetrical [3], yet presenting a good crystalline organization. Thanks to a combination of experimental analysis and theoretical symmetry analysis, a unified description of the observed morphologies (Fe-Au and Fe-AuAg systems) is proposed, whatever their symmetry [4]. First the crystal lattice accommodation is comprehensively analyzed from the experimental Fe-AuAg system. The two possible bcc-fcc epitaxial relationships generate a core-shell interface in the shape of a truncated rhombic dodecahedron. This results in two different types of grains in the shell which are elastically accommodated between them by an equal distribution of twins and low angle grain boundaries. At the same time, a symmetry breaking results from two possible growth variants originating from the Nishiyama-Wasserman epitaxial relationships. The shell grains fit together in a nano-puzzle-like organization, resulting in a large number (186 in theory) of possible arrangements distributed in 13 different point groups of symmetry ( $m\bar{3}$ ,  $4/m$  and their sub-groups), all of lower order than the  $m\bar{3}m$  cubic symmetry of the core. If the variants are randomly distributed, the probability for the NP to be asymmetric (group 1) is 80%. Extending this approach to other core shapes succeeds in predicting dissymmetrical or dramatically off-centered morphologies experimentally observed in Fe-Au NPs [3]. This analysis highlights that in these bcc@fcc systems (and in similar polycrystalline nanostructures), not only a NPs population presents a size and eventually composition distribution, but it also could present a distribution of symmetry and a distribution of morphologies, even with a perfectly symmetric core. The studied system is a case study illustrating the powerfulness of reasoning by symmetry to predict the morphology variability.

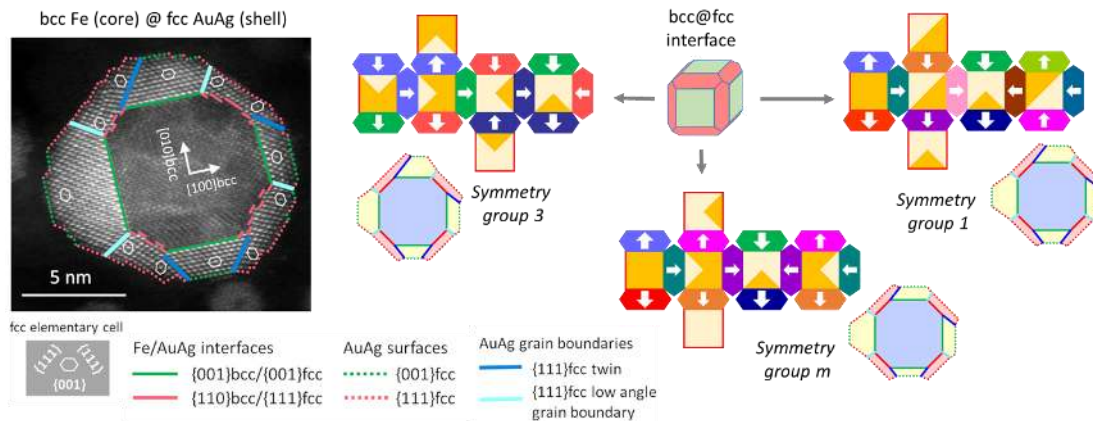


Fig.1 : Crystallographic analysis of a Fe@AuAg NP, observed along a  $\langle 001 \rangle$  direction of the Fe core, and scheme of some possible 3D morphologies for this NP [4].

[1] P. Benzo, S. Combettes, B. Pecassou, N. Combe, M. Benoit, M. Respaud, and M. J. Casanove, Phys. Rev. Mater. 3, 096001 (2019)

[2] A. Ponchet, S. Combettes, P. Benzo, N. Tarrat, M.J. Casanove, M. Benoit, J. Appl. Phys. 128, 055307 (2020)

[3] S. Combettes, T. Hungria, S. Barre, B. Pecassou, R. Cours, M. Benoit, M.-J. Casanove, A. Ponchet, and P. Benzo - Eur. Phys. J. Appl. Phys. 97, 27 (2022) [hal-03685120](https://doi.org/10.1051/epjap/20229727)

[4] A. Ponchet, N. Tarrat, T. Hungria, M. Benoit, M.J. Casanove, P. Benzo, J. Appl. Phys. (2023) in press.

## Iron Garnet Heteroepitaxial Film Synthesis

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Yttrium Iron Garnet (YIG –  $\text{Y}_3\text{Fe}_5\text{O}_{12}$ ) and Thulium Iron Garnet (TmIG –  $\text{Tm}_3\text{Fe}_5\text{O}_{12}$ ) films 3 to 100 nm-thick were deposited on Gadolinium Gallium Garnet (GGG -  $\text{Gd}_3\text{Ga}_5\text{O}_{12}$ ) (111) and substituted GGG (sGGG) (111) substrates at room temperature using the radio frequency sputtering technique. They were annealed in air after deposition. In the previous works iron garnets thin films were mostly grown by pulsed laser deposition (PLD), which is an interesting technique for growing complex polycationic films but limits the area of growth and can cause particulate incorporation in ablated films and non-uniform deposition [1, 2]. On the contrary, the sputtering deposition technique has the advantage of allowing the fast growth of uniform heterostructures on large wafers and is compatible with lithography tools.

The structural properties of iron garnets were studied using X-ray reflectivity (XRR) and X-ray diffraction (XRD) techniques. The simulations of the XRR curves were performed using LEPTOS software, which demonstrated low roughness in the range of 0.5 nm for all iron garnet samples, and the estimated thicknesses were close to the nominal values, based on the deposition time (Fig. 1a).

In the XRD diagrams, only (hhh) peaks are evidenced in the  $\theta - 2\theta$  geometry. Laue oscillations around the film (444) diffraction line demonstrate the crystalline coherence across the film thickness (Fig. 1b). The out-of-plane strain of the TmIG on GGG sample is  $\varepsilon=0,49\%$ , caused by the difference in lattice parameters of TmIG and GGG. It induces a perpendicular magnetic anisotropy in the sample. The YIG/GGG is not strained epitaxially due to lattice quasi-match.

The strain coefficient assuming in-plane heteroepitaxy of  $\varepsilon=0,99\%$  was estimated for TmIG/SGGG, it is  $\approx 0,5\%$  lower than if it would be in the case of complete epitaxial strain, meaning that the TmIG layer is not fully strained or is partially relaxed. On the contrary, the measured strain for YIG/SGGG  $\varepsilon=0,96\%$  is relatively close to the value in the full strain case and YIG becomes perpendicularly magnetised.

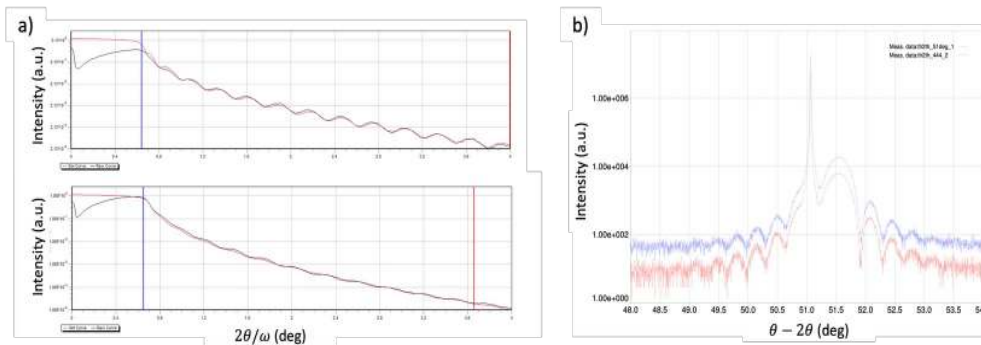


Fig.1. a) XRR oscillations (black line) of TmIG(30 nm)/GGG samples annealed at 800°C (upper) and 900°C (lower) and simulation curve (red lines); b) XRD diagram of TmIG(30 nm)/GGG (444) line in  $\theta - 2\theta$  geometry.

The authors would like to thank LANEF and Nanosciences Foundation for financial support of this work.

[1] C.O. Avci *et al.*, Nature Nanotechnology **14**, 561-566 (2019).

[2] S. Vélez *et al.*, Nature Communications **10**, 4750 (2019).

# Nanoparticules, catalyse

# Role of Dimensionality and Size in Controlling the Drag Seebeck Coefficient of Doped Silicon Nanostructures: A Fundamental Understanding

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In this theoretical study [1] we examine the influence of dimensionality, size reduction, and heat-transport direction on the phonon-drag contribution to the Seebeck coefficient of silicon nanostructures. Phonon-drag contribution, which arises from the momentum transfer between out-of-equilibrium phonon populations and charge carriers, significantly enhances the thermoelectric coefficient. Our implementation of the phonon drag term accounts for the anisotropy of nanostructures such as thin films and nanowires through the boundary- and momentum-resolved phonon lifetime. Our approach also takes into account the spin-orbit coupling which turns out to be crucial for hole transport. We reliably quantify the phonon drag contribution at various doping levels, temperatures, and nanostructure geometries for both electrons and holes in silicon nanostructures. Our results support the recent experimental findings, showing that a part of phonon drag contribution survives in 100 nm silicon nanostructures.

## Acknowledgements:

Calculations have been performed with the Quantum ESPRESSO [2], EPW [3], D3Q [4] and the Wannier90 code. This work has been granted access to HPC resources by the French HPC centers GENCI (Project 2210). Financial supports from the ANR (PLACHO project ANR-21-CE50-0008, Macacqui flagship Labex Nanosacly ANR-10-LABX-0035), from the DIM SIRTEQ, from the CNRS-CEA program "Basic research for energy" are gratefully acknowledged.

## References:

- [1] R. Sen, N. Vast, J. Sjaskte, Phys. Rev. B Letters **08**, L060301 (2023).
- [2] P. Giannozzi et al., Advanced capabilities for materials modelling with QUANTUM ESPRESSO. J. Phys.: Condens. Matter **29**, 465901 (2017).
- [3] S. Ponce, E. R. Margine, C. Verdi, and F. Giustino. EPW: Electron-phonon coupling, transport and superconducting properties using maximally localized Wannier functions. Comp. Phys. Comm. **209**, 116 (2016).
- [4] L. Paulatto, F. Mauri, and M. Lazzeri, Anharmonic properties from a generalized third-order ab initio approach: Theory and applications to graphite and graphene. Phys. Rev. B **87**, 214303 (2013).

## Work function measurements of materials exposed to hydrogen plasmas, correlation with the negative ion surface production efficiency

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This work deals with the production of negative-ions on HOPG and C12A7 electrified /1/ surfaces exposed to low pressure deuterium plasmas ( $P=2\text{Pa}$ ). The aim is to enable the development of cesium-free negative-ion sources, which would be valuable for many applications, microelectronics processing, ions thrusters and neutral beam injectors for future nuclear fusion reactors.

Negative-ion surface production in plasma is relying on the backscattering of an incoming hydrogen particle or the sputtering of an adsorbed one, together with the capture of an electron on the surface. The surface ionization probability describes the probability that a backscattered or a sputtered hydrogen particle is negatively ionized.

This probability is strongly depending on the surface work-function for metallic surfaces and on the ionization energy and gap width for semi-conductive or insulating surfaces. The present work is devoted to study the negative ion formation ( $\text{H}^-$ ,  $\text{D}^-$ ) at the surface of different materials in correlation with the evolution of their surface electronic properties upon hydrogen (Deuterium) plasma exposure. For this purpose, we have developed a photoemission yield spectroscopy (PYS) original diagnostic that allows us to measure in-situ the ionisation energy after plasma exposure. We combine PYS and the Fowler method to determine the insulating or metallic character of plasma-exposed HOPG, Diamond, C12A7 electrified and Gadolinium. We show that the surface electronic properties strongly evolve as a function of the plasma exposure experimental conditions (positive ion energy, surface temperature...) and correlate those changes with the evolution of the negative-ion yields.

1 . Sasao, R. Moussaoui, D. Kogut, J. Ellis, G. Cartry, M. Wada, K. Tsumori, and H. Hosono. Negative-hydrogen-ion production from a nanoporous  $12\text{CaO} \cdot 7\text{Al}_2\text{O}_3$  electrified surface. Applied Physics Express, 11(6), 2018. ISSN 18820786. doi:[10.7567/APEX.11.066201](https://doi.org/10.7567/APEX.11.066201).

# Matière molle



## Etude de l'interface Liquide Ionique/Oxyde de Graphène

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Les supercondensateurs à base d'électrolyte en liquide ionique (LI) et d'électrode en graphène ou d'oxyde de graphène (GO) sont des dispositifs prometteurs pour le stockage d'énergie (haute capacité, charge rapide, haute densité de puissance...). Ils présentent cependant une densité d'énergie limitée en raison de la faible surface d'interaction entre l'électrolyte et l'électrode, d'où la nécessité d'étudier cette interface. Nous avons choisi la stratégie des films de Langmuir pour former des interfaces IL/GO facilement accessibles. Nous avons réalisé des films mixtes composés de LI ([C20mim]<sup>+</sup>[NTf2]<sup>-</sup>) et GO sur surface liquide que nous avons étudiés par isothermes, BAM, réflectivité (XRR) et diffraction rasante des rayons X (GIXD), puis par AFM après transfert sur substrat solide. Les résultats montrent que la structure de l'interface IL/GO est déterminée non seulement par les conditions thermodynamiques du film (pression superficielle, concentration), mais également par la nature de l'interface «opposée». En effet, leur interprétation indique que, pour toutes les pressions de surface, les feuillets de GO se placent au-dessus des domaines de molécules de LI en contact avec la phase aqueuse qui forment une monocouche désordonnée. Si la pression augmente au-delà du collapse, des molécules de LI recouvrent l'autre face des feuillets de GO. De ce côté (au contact de l'air), les molécules sont soit allongées parallèlement à la surface du feuillet (à faible densité surfacique) soit perpendiculaires et organisées sur un réseau 2D si leur densité est suffisante [1]. La monocouche de LI intercalée entre la phase aqueuse et les feuillets reste en revanche désordonnée pour toute les pressions de surface. Ces résultats indiquent un scénario complexe par rapport à ceux obtenus à partir des simulations [2].

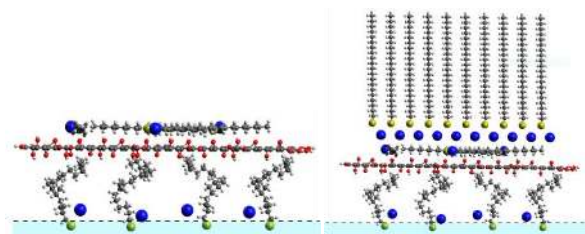


Schéma des interfaces entre le liquide ionique C20<sub>mim</sub> (gris et vert) - NTF<sub>2</sub> (bleu) et un feuillet d'oxyde de graphène (gris et rouge) à faible (à gauche) et haute (à droite) densité de surface. La position des NTF<sub>2</sub> est arbitraire.

[1] H. Ibrahim, PhD Thesis, Sorbonne Université 2020 and H. Ibrahim et al submitted to Langmuir (2022)

[2]. Behnoosh Sadeghi Moghadam et al. Physical Chemistry Chemical Physics 2016 **18**.48 33053-33067

# Modèle physique apportant un nouvel éclairage sur les interactions complexes entre les molécules membranaires

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...

## 1 Introduction

Du fait de leur organisation et des fonctions multiples qui leur sont conférées par leur structure complexe [2], les membranes cellulaires présentent un intérêt à la fois fondamental et applicatif mais leur approche nécessite souvent une approche interdisciplinaire combinant outils mathématiques et physiques et connaissances biologiques. Reflet de cette complexité, l'élucidation de la relation entre leurs structures et leurs fonctions multiples se heurte à des obstacles majeurs. D'origine structurale et fonctionnelle, la complexité des membranes biologiques résulte d'un vaste ensemble d'interactions moléculaires s'exprimant dans les processus biologiques mais aussi de l'exploitation de couplages naturels entre divers mécanismes physico-chimiques. De nombreux modèles relevant de la Biophysique visent une description mécanique et thermodynamique de ces membranes s'appuyant sur la fameuse fonctionnelle (énergie) de Canham-Helfrich [3, 5, 20], prenant en compte la forme, c'est-à-dire la géométrie et la topologie des membranes et permettant la détermination des configurations d'équilibre des membranes. Du point de vue mécanique, ces membranes présentent les caractéristiques combinées de solides et de fluides (écoulement interne à la membrane comme évoqué dans le vieux modèle de la mosaïque fluide [3]). L'étude présentée ici concerne un modèle mécanique simple de membranes cellulaires planes ou courbées et permettant de décrire les interactions induites entre protéines incluses dans celle-ci [14, 15]. Basé sur une extension simple de la fonctionnelle de Helfrich, le modèle décrit d'abord la dynamique déterministe des déplacements normaux de membranes élastiques homogènes et isotropes [1, 6, 16]. Le spectre des excitations de basse énergie (ondes de courbure) est discuté dans le cas de membranes de haute symétrie telles les vésicules sphériques ainsi que la forme générale de la compliance de celles-ci [7, 8, 9]. Dans une seconde étape, la théorie générale des fluctuations thermiques [4] de la membrane est présentée ainsi que ses effets sur les interactions résiduelles entre protéines incluses, de nature entropique [13, 17, 18]. La forme du potentiel d'interaction correspondant est calculée numériquement dans le cas de membranes planes. Le rôle potentiel de ces interactions sur l'organisation des protéines au sein de la membrane est discuté. Leurs réorganisations au sein de la membrane pourraient être approchées efficacement comme transitions de phases de la membrane 'habillée' par une analogie intéressante de notre modèle avec le gaz de Coulomb 2D.

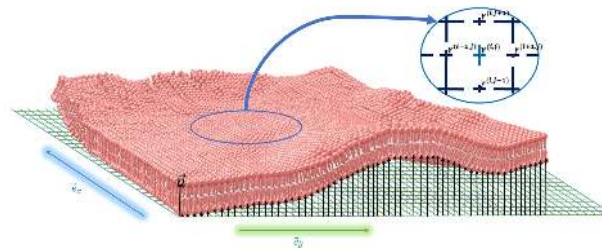


FIGURE 1 – Représentation schématique d'une membrane cellulaire courbée

**Mots clefs :** Membrane cellulaire ; Helfrich ; Courbure ; Fluctuations thermiques ; mouvement aléatoire

## Références

- [1] ORSI, Mario, HAUBERTIN, David Y., SANDERSON, Wendy E., et al. A quantitative coarse-grain model for lipid bilayers. *The Journal of Physical Chemistry B*, 2008, vol. 112, no 3, p. 802-815.
- [2] BENGA, Gheorghe et HOLMES, Ross P. Interactions entre les composants des membranes biologiques et leurs implications pour la fonction membranaire. *Progrès de la biophysique et de la biologie moléculaire*, 1984, vol. 43, n° 3, p. 195-257.
- [3] SEIFERT, Udo. Configurations of fluid membranes and vesicles. *Advances in physics*, 1997, vol. 46, no 1, p. 13-137.
- [4] PROST, J. et BRUINSMA, R. Shape fluctuations of active membranes. *Europhysics Letters*, 1996, vol. 33, no 4, p. 321.
- [5] HELFRICH, Wolfgang. Elastic properties of lipid bilayers : theory and possible experiments. *Zeitschrift für Naturforschung c*, 1973, vol. 28, no 11-12, p. 693-703.
- [6] DEVAUX, Philippe F. Static and dynamic lipid asymmetry in cell membranes. *Biochemistry*, 1991, vol. 30, no 5, p. 1163-1173.
- [7] HENLE, Mark L., MCGORTY, R., SCHOFIELD, Andrew B., et al. The effect of curvature and topology on membrane hydrodynamics. *Europhysics Letters*, 2008, vol. 84, no 4, p. 48001.
- [8] RÓŻYCKI, Bartosz et LIPOWSKY, Reinhard. Spontaneous curvature of bilayer membranes from molecular simulations : Asymmetric lipid densities and asymmetric adsorption. *The Journal of chemical physics*, 2015, vol. 142, no 5, p. 02B601-1.
- [9] SREEKUMARI, Aparna et LIPOWSKY, Reinhard. Lipids with bulky head groups generate large membrane curvatures by small compositional asymmetries. *The Journal of Chemical Physics*, 2018, vol. 149, no 8, p. 084901.
- [10] CAMPELO, Felix, FABRIKANT, Gur, MCMAHON, Harvey T., et al. Modeling membrane shaping by proteins : focus on EHD2 and N-BAR domains. *FEBS letters*, 2010, vol. 584, no 9, p. 1830-1839.
- [11] CAMPELO, Felix et KOZLOV, Michael M. Sensing membrane stresses by protein insertions. *PLoS computational biology*, 2014, vol. 10, no 4, p. e1003556.
- [12] FARSAAD, Khashayar et DE CAMILLI, Pietro. Mécanismes de déformation membranaire. *Opinion actuelle en biologie cellulaire*, 2003, vol. 15, n° 4, p. 372-381.
- [13] ARANDA-ESPINOZA, Helim, BERMAN, A., DAN, Nily, et al. Interaction between inclusions embedded in membranes. *Biophysical journal*, 1996, vol. 71, no 2, p. 648-656.
- [14] MAHATA, Paritosh, SINGHAL, Lakshya, PRASAD, Ravi Kant, et al. Computational investigation for deformation of lipid membrane by BAR proteins due to electrostatic interaction. *Materials Today : Proceedings*, 2022, vol. 61, p. 1-9.
- [15] ZHOU, Y. C., ARGUDO, David, MARCOLINE, Frank V., et al. A computational model of protein induced membrane morphology with geodesic curvature driven protein-membrane interface. *Journal of computational physics*, 2020, vol. 422, p. 109755.
- [16] DASGUPTA, Anirvan et TAMADAPU, Ganesh. In-plane dynamics of membranes having constant curvature. *European Journal of Mechanics-A/Solids*, 2013, vol. 39, p. 280-290.
- [17] KIM, K. S., NEU, John, et OSTER, George. Curvature-mediated interactions between membrane proteins. *Biophysical journal*, 1998, vol. 75, no 5, p. 2274-2291.
- [18] DAN, Nily. Membrane-induced interactions between curvature-generating protein domains : the role of area perturbation. *AIMS Biophysics*, 2017, vol. 4, no 1, p. 107-120.
- [19] BRANNIGAN, Grace, LIN, Lawrence C.-L., et BROWN, Frank LH. Implicit solvent simulation models for biomembranes. *European Biophysics Journal*, 2006, vol. 35, p. 104-124.
- [20] CANHAM, Peter B. The minimum energy of bending as a possible explanation of the biconcave shape of the human red blood cell. *Journal of theoretical biology*, 1970, vol. 26, no 1, p. 61-81.

# Nano-lithography with high- $\chi$ block copolymers: interplay between self-organization and dewetting kinetics

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The directed self-assembly (DSA) of block copolymers (BCPs) is a powerful method with the potential to enable the manufacture of high-resolution (sub-10 nm) features in microelectronics. Nevertheless, several critical challenges remain, including the control of the polymer layer dewetting. Indeed, ultrathin films of high- $\chi$  BCPs ( $\chi$  being the Flory-Huggins interaction parameter between the BCP blocks) deposited on or between neutral surfaces (to promote a perpendicular orientation of the nano-features, as depicted in Fig. 1a) are thermodynamically unstable. Without external constraints, such as a rigid top layer (commonly referred to as a top-coat, TC), these films tend to undergo dewetting [1]. So far, the dewetting of high- $\chi$  BCPs is a phenomenon not yet fully understood or controlled. There exist various theories regarding its kinetics, particularly when compared to the self-assembly kinetics. Furthermore, dewetting is typically viewed as an undesired occurrence and is seldom leveraged to construct more intricate designs that would otherwise be unattainable through conventional DSA methods.

The interplay between dewetting and microphase separation kinetics remains poorly understood, and it's unclear what factors determine the relative rates of these two phenomena. Therefore, this work aims at better understanding the coupling between these processes by designing an experimental framework that enables simultaneous control of BCP phase separation and dewetting. In this study, we designed a platform based on a BCP layer sandwiched between a neutral polymer brush layer and a functional TC, enabling controlled crosslinking and photo-patterning of the TC layer. This patterning allows for the creation of patterns with BCP located both beneath a crosslinked TC and exposed to air (Fig. 1b). During thermal annealing, the BCP begins to self-assemble and dewet, resulting in both phenomena coexisting in two different regions of the sample, albeit with varying degrees of intensity (Fig. 1c)).

Another important aspect of the dewetting is that it can be harnessed both to guide the assembly of the block copolymer [2] or to generate various patterns, such as ordered droplets [3]. The same experimental platform also facilitates the investigation of the diverse shapes adopted by the BCP layer during the dewetting process within constrained spaces of varying geometries.

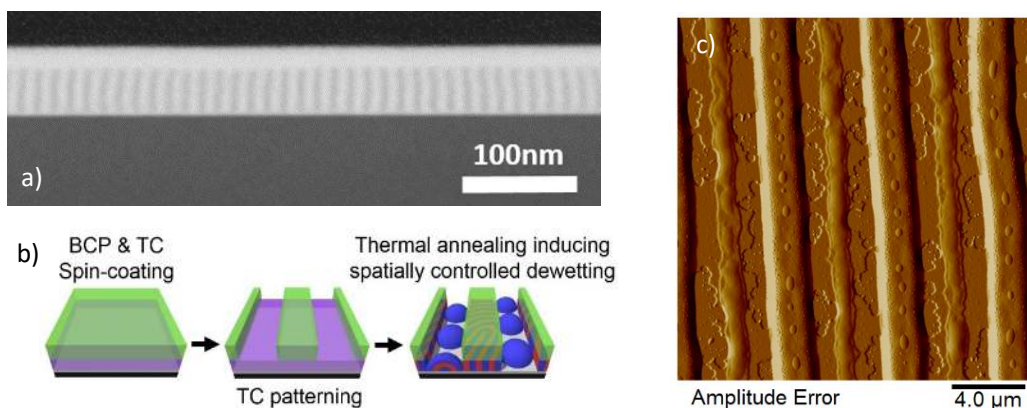


Fig.1. a) STEM cross-section of vertically-aligned 9-nm resolution polymer lamellas on flat surfaces; b) Representation of possible design; c) AFM topography of an initial sample with line-space pattern.

- [1] X. Chevalier et al., *Nanotechnology*, 34, 175602 (2023).
- [2] H. Zhang et al. *Macromolecules*, 53, 21, 9631-9640 (2020)
- [3] F. F. Lupi et al., *ACS Nano*, 12, 7, 7076–7085 (2018)

# Magnétisme

## Interacting magnetic adatoms and clusters: Dy/HOPG

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We study graphene-mediated magnetic interaction between Dy adatoms and clusters adsorbed on HOPG (highly oriented pyrolytic graphite) by combining STM, X-ray absorption spectroscopy (XAS) and X-ray magnetic circular dichroism (XMCD).

Our STM studies show, for the relevant coverage of about 1% of a monolayer, the coexistence of adatoms and small clusters. From statistical analysis we determine the abundance of monomers and clusters, the direct capture area of monomers, as well as the distance distributions. For a deposition temperature of 10 K we find statistical growth, while deposition at 40 – 60 K leads to regularly spaced atoms suggesting repulsive electrostatic interactions caused by charge transfer between adatoms and substrate.

XAS measurements reveal that Dy atoms inside clusters are trivalent whereas the adatoms are divalent. This allows XMCD measurements of  $M(H)$ -curves for each species. We find that the clusters are paramagnetic, while the monomer magnetic moments are anti-parallel to the external magnetic field  $H$  for  $\mu_0 H$  smaller than 3 T. This magnetic behavior differs from the one obtained on Dy/graphene/Ir(111) which show several steps in the  $M(H)$  curves, previously explained with magnetic level crossings [1,2]. In addition, the monomers exhibit slow magnetic relaxation resulting in hysteretic behavior. These data reveal antiferromagnetic coupling between monomers and clusters on HOPG.

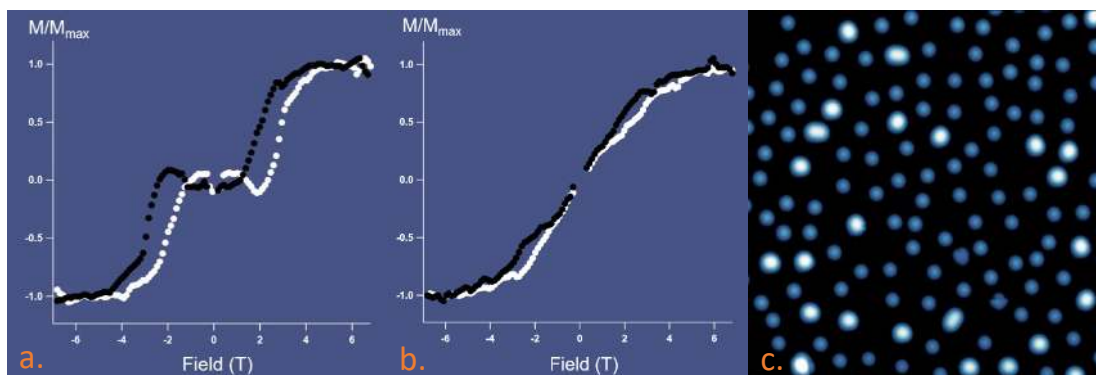


Fig.1 (a) XMCD  $M(H)$  curves of Dy/HOPG for divalent atoms (2T/min, 2.5K) black dots representing the positive to negative field and white the contrary. (b) Same curves for trivalent atoms inside clusters. (c) STM image of 1% ML Dy/HOPG showing adatoms and clusters of Dy (10 pA, -300 mV, 5K, 30 x 30nm)

[1] R. Baltic et al., Nano Lett. **16**, 7610 (2016).

[2] A. Curcella et al., Phys. Rev. Lett. **130**, 106702 (2023).



# Electric field manipulation of magnetic properties of Pt/Co/oxide thin films

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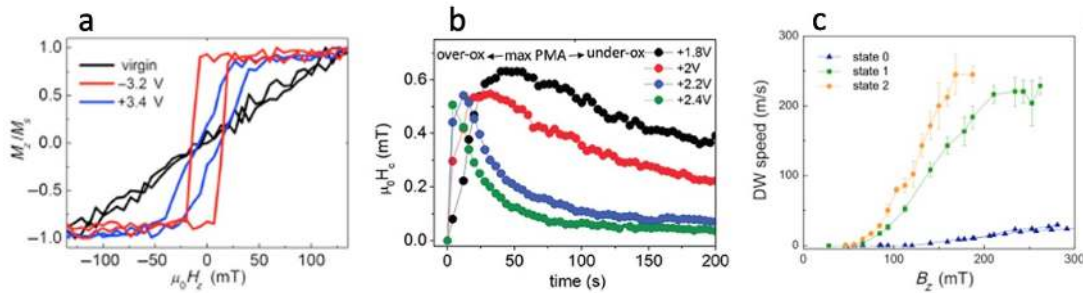
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The manipulation of magnetism with a gate voltage, and in particular by magneto-ionics - where the magnetization is controlled by an electric field driving the migration of ionic species - is a fast developing research field which opens the perspective of energy efficient magnetic devices. Magnetoionic effects under micropatterned electrodes in solid-state devices allow modifying magnetic properties locally, in a nonvolatile and reversible way. In this work, we illustrate some of the results obtained on Pt/Co/oxide thin films using HfO<sub>2</sub> or ZrO<sub>2</sub> thin layer as a solid state ionic conductor. We demonstrate that tuning magnetic anisotropy, magnetization and Dzyaloshinskii-Moriya interaction allows modifying “at will” the dynamics of nontrivial magnetic textures such as skyrmions and chiral domain walls. Through x-ray photoelectron spectroscopy measurements, we show that the change of magnetic properties can be directly attributed to the modification of the oxidation state of the ferromagnetic layer via electric field driven oxygen ion migration.



**Figure 1.** (a) Polar Kerr hysteresis loops showing the electric field induced reversible change of easy axis magnetization from in plane to out-of-plane in Pt/Co/TbOx thin films [1]; (b) time-dependence of the magnetic anisotropy with applied gate voltage [2]; Electric-field induced variation of chiral domain wall dynamics in Pt/Co/Tb/AlOx thin films [3].

[1] A. Fassatoui et al. Phys. Rev. Applied 14, 064041 (2020)

[2] A. Fassatoui et al. Small 2021, 2102427

[3] C. Balan et al. 18, 034065 (2022)

## Control of hybrid organic/inorganic interfaces: growth and multi-scale characterizations in magnetic tunnel junctions

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The use of organic tunnel barriers in spintronic devices is multiple: low cost, flexibility and long spin lifetime [1, 2]. In the context of molecular spintronics, the study of organic/inorganic ferromagnetic metal interfaces is promising, in particular due to the spin-dependent hybridized interface states that can enhance or modify the magnetoresistance effect. The study of spin tailoring at hybrid interfaces is called spinterface [3]. Indeed, electronic properties at metal/organic interface strongly depend on the quality of the interface. In this work, we will present complementary multi-scale characterizations used to each step of heterostructure's growth under ultra-high vacuum environment. In particular, by using BEEM (Ballistic Electron Emission Microscopy), a technique derived from the Scanning Tunneling Microscopy one [4, 5], it is possible to image buried interfaces, with a sub-nanometer resolution, thus detecting any pinhole [6]. By recording BEEM current versus hot-electron energy, a local electronic band structure can be determined. Here we will present results obtained on a ferromagnetic Co top-contact deposited on a 1-hexadecanethiol monolayer grafted on GaAs(001). Results at buried interfaces are discussed for various deposition methods of the Co top-contact. We will show that optimized Co top contact deposition by a soft-landing method [7, 8] allows the preparation of homogeneous magnetic tunnel junctions free of pinholes over several square micrometers.

[1] J. R. Petta, S. K. Slater, et al., *Physical Review Letters*, **93**, 136601 (2004)

[2] S. Sanvito, *Chemical Society Reviews*, **40**, 3336-3355 (2011)

[3] S. Sanvito, *Nat Phys*, **6**, 562-564 (2010)

[4] W. J. Kaiser, L. D. Bell, *Phys. Rev. Lett.*, **60**, 1406 (1988)

[5] L. D. Bell, W. J. Kaiser, *Phys. Rev. Lett.*, **61**, 2368 (1988)

[6] A. Junay, S. Guézo, et al., *Journal of Applied Physics*, **118**, 085310 (2015)

[7] M. M. Maitani, D. L. Allara, et al., *Applied Physics Letters*, **96**, 173109-3 (2010)

[8] A. Junay, S. Guézo et al., *The Journal of Physical Chemistry C*, **120**, 24056 (2016)

# Tuning Perpendicular Magnetic Anisotropy in TmIG/YIG/GGG bilayers

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Magnetic skyrmions are local whirling of the magnetization found in certain chiral magnetic films with properties including topological stability, sizes down to nm-scale and the possibility of manipulation by electrical current [1]. The heterostructures composed of ferrimagnetic oxides (FMOx) based on rare-earth iron garnets in contact with high spin-orbit materials (SOM) have recently attracted a large attention due to their assets for the current induced skyrmion manipulation. Their advantages include electrical insulation which allows to minimize the energy loss due to current shunting, small saturation magnetization  $M_s$ , small magnetic damping  $\alpha$ , leading to large domain wall mobility, significant DMI interaction at the FMOx/SOM interface [2].

The Thulium Iron Garnet (TmIG –  $Tm_3Fe_5O_{12}$ ) and Yttrium Iron Garnet (YIG –  $Y_3Fe_5O_{12}$ ) samples with thicknesses varying from 3 to 100 nm were deposited on Gadolinium Gallium Garnet (GGG -  $Gd_3Ga_5O_{12}$ ) (111) substrate using radio frequency sputtering technique and were annealed in air after deposition. TmIG/GGG samples have perpendicular magnetic anisotropy (PMA) for all thicknesses ranging between 3 and 40 nm with square hysteresis loop and sharp reversal associated with large magnetic domains.

With the purpose to significantly reducing the magnetic anisotropy of the films and tune it close to the out-of-plane – in-plane transition, the bilayers TmIG/YIG/GGG with fixed TmIG layer thickness  $t_{TmIG} = 10$  nm and different  $t_{YIG}$  were fabricated. Considering the effective anisotropy coefficient  $K_{eff} = \frac{1}{2}\mu_0 M_s H_{sat}$ , where  $M_s$  is the magnetization and  $H_{sat}$  is the saturation field, obtained from SQUID measurements, the model of the bilayer effective anisotropy was developed, dependent on effective anisotropies of TmIG and YIG layers  $K_{TmIG}$  and  $K_{YIG}$ . The layer  $t_d = 2$  nm is considered as non-magnetic between YIG layer and GGG substrate (Fig. 1a).

The MOKE measurements demonstrated that TmIG/YIG samples with effective anisotropy  $K_{eff} < 1$  kJ/m<sup>3</sup> have low remanence hysteresis cycle (Fig. 1b) and small magnetic domains (down to 1  $\mu$ m) are observed (Fig. 1c).

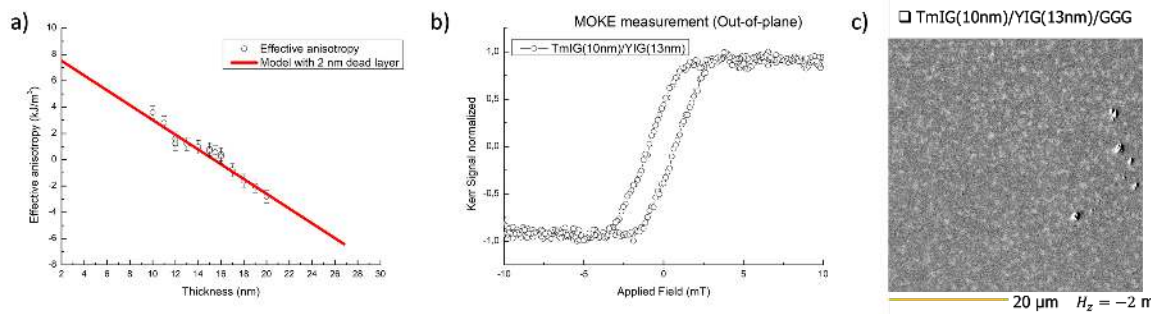


Fig. 1. a) Dependence of the  $K_{eff}$  on YIG layer thickness in TmIG(10 nm)/YIG( $t_{YIG}$  nm)/GGG samples, fitted with the model; b) TmIG(10 nm)/YIG(13 nm)/GGG hysteresis cycle with low remanence; c) the polar-MOKE image of TmIG(10 nm)/YIG(13 nm)/GGG sample in the applied out-of-plane field  $H_z$ .

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[1] O. Boulle *et al.*, Nature Nanotechnology **11**, 449-454 (2016).

[2] L. Caretta *et al.*, Nature Communications **11** (2020).

## Out-of-plane antiferromagnetic spins induced by spin-reorientation transition in NiO(111)/Co bilayers

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A lot of extensive research has been focused in the past, as well as nowadays, on the engineering of magnetic anisotropy in ferromagnetic (FM) specimens. However, this attention has been shifted onto, among others, antiferromagnetic (AFM) materials, which turned out to be promising spintronics candidates, hence, giving birth to AFM spintronics. The main goal of AFM spintronics is to supplement or even potentially substitute FMs in microelectronic devices. One of the most well-known AFMs is nickel oxide – NiO, which stands out for its significantly high Néel temperature and the ease with which it allows the manipulation of the in-plane [1] antiferromagnetic spins through the coupling with an FM, making it a promising contender for practical applications.

To investigate the polar spin-reorientation transition (SRT) in the NiO(111)/Co epitaxial bilayer, we have employed Kerr microscopy and X-ray Magnetic Linear and Circular Dichroism (XMLD, XMCD) spectroscopies at the PIRX end-station of The National Synchrotron Radiation Centre SOLARIS. The acquired XMCD spectra, as well as Kerr microscopy results, of Co grown epitaxially on Au(111)/W(110) directly confirmed a shift from an in-plane to out-of-plane SRT [2] as the thickness of Co decreased. Similarly, the XMLD spectra at the L<sub>2</sub> absorption edge of NiO revealed that as the Co thickness decreases below the critical Co SRT thickness ( $d_{Co} = 15 \text{ \AA}$ ), the spins of the antiferromagnetic nickel oxide transitioned to an out-of-plane orientation.

The observed polar SRT in the antiferromagnetic NiO arises most likely due to the AFM/FM proximity effect, a consequence of the strong interfacial exchange coupling [3].

[1] Ślęzak, M., Nayef, H., Drozd, P., Janus, W., Koziol-Rachwał, A., Szpytma, M., Zając, M., Menteş, T.O., Genuzio, F., Locatelli, A., Ślęzak, T., **Physical Review B** **104**, **134434**, *Controllable magnetic anisotropy and spin orientation of a prototypical easy-plane antiferromagnet on a ferromagnetic support* (2021).

[2] Stupakiewicz, A., Maziewski, A., Matlak, K., Spiridis, N., Ślęzak, M., Ślęzak, T., Zając, M., Korecki, J., **Physical Review Letters** **101**, **217202**, *Tailoring of the perpendicular magnetization component in ferromagnetic films on a vicinal substrate* (2008).

[3] Ślęzak, M., Drózd, P., Janus, W., Nayef, H., Koziol-Rachwał, A., Szpytma, M., Zając, M., Menteş, T. O., Genuzio, F., Locatelli, A., Ślęzak, T., **Nanoscale** **12**, **18091-18095**, *Fine tuning of ferromagnet/antiferromagnet interface magnetic anisotropy for field-free switching of antiferromagnetic spins* (2020).

STM, transport, optique

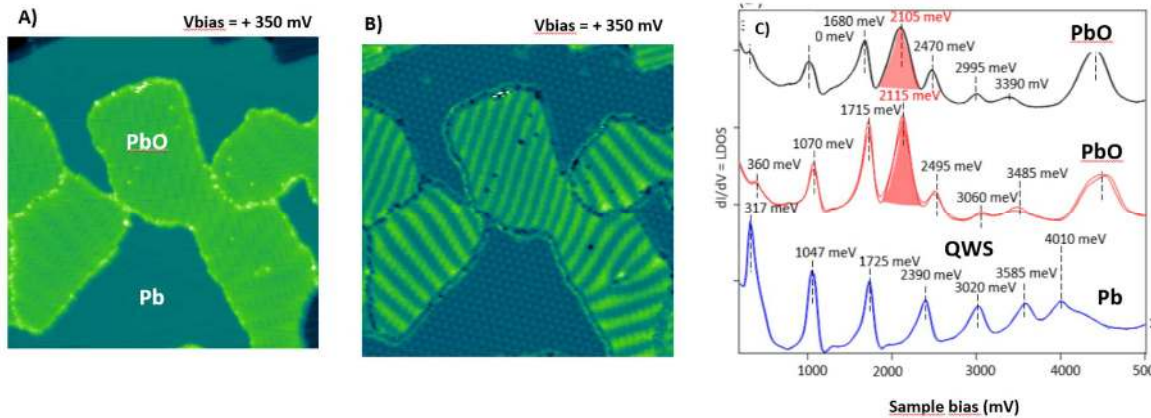
# Quantum well states and electron interferometry in ultrathin films of Pb on Ag(111) as a probe of buried interfaces

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Electron confinement in thin metallic films has been intensively studied theoretically [1] and experimentally from both ARPES experiments [1,2] and STM/STS [3,4]. In some cases, the quantum resonances that develop in the film can be used to study the buried interfaces reflecting electrons that propagate in the direction perpendicular to the film [5]. It has been shown that structural information on the buried interface as deep as 100 nm can be obtained by mapping the LDOS at the surface of the film [6]. In this communication we report some results on the quantum well states that develop in thin Pb films deposited on Ag(111). We will show how a thin layer of PbO, grown on the top of the film, modify the reflection properties of electrons. Depending on the local arrangement between the atomic lattices of Pb and PbO various moiré patterns are observed in the Local Density Of States (LDOS) at the surface of the film as observed by STS. The buried atomic arrangement at the Pb/Ag interface is also revealed in the surface LDOS.



**Fig.1.** A) STM image (Z channel) of single layer PbO islands grown on the top of a thin Pb/Ag(111) film. – B) LDOS map on the same area showing a 1D moiré pattern on the PbO islands and originating from the Pb/PbO interface and a 2D moiré pattern on the top of the Pb film due to the buried Pb/Ag(111) interface. - C) LDOS spectra recorded on the top of PbO islands (red and black) and on the top of the Pb film (bleue)

- [1] T.-C. Chiang, Surf. Sci. Rep. **39**, 181 (2000).
- [2] N J Speer et al. - Science, 314, 804 (2006).
- [3] M. Becker and R. Berndt - Phys. Rev. B **81** (2010)
- [4] M.C.Yang et al. – Phys.Rev. Lett **102** (2009) 196102
- [5] I.B. Altfeder et al. – Phys. Rev. Lett. **80** (1998) 4895
- [6] Kurnosikov O.et al. Nanoscale Horizons **8** (2023) 900-911.



# Physique-chimie des surfaces

# Nanobeam soft X-ray microscope to unveil nanocrystals-based device energy landscape

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As the field of nanocrystal-based optoelectronics continues to advance, the need for more sophisticated techniques to uncover the electronic structure of nanocrystals under device-relevant conditions has become increasingly apparent<sup>1</sup>. Conventional spectroscopic methods often focus on pristine materials, overlooking the critical factors such as the interaction of the active material with its surrounding environment, including transport layers and electrodes, the impact of applied electric fields, and possible illumination effects. Therefore, it is imperative to develop tools capable of probing devices *in situ* and *operando*. Here, we introduce a novel approach that leverages nanobeam scanning soft X-ray photoemission microscopy, specifically, to elucidate the energy landscape of nanocrystal-based devices with an impressive spatial resolution of less than 1  $\mu\text{m}$ . This method offers remarkable versatility, making it applicable to a wide range of device geometries, including Field Effect Transistors (FETs)<sup>2</sup>, photoconductive device<sup>3</sup>, photodiodes<sup>4</sup> and even complex focal plane arrays (FPA)<sup>5</sup>. Using this technique, we can directly quantify the diode's built-in voltage, and through *operando* measurements, we can uncover the effects of applied drain and gate electric fields. Furthermore, beyond probing the energy landscape under biasing conditions, we gain valuable insights into the vectorial distribution of the electric field within the operating device. This breakthrough in nanobeam soft X-ray microscopy significantly enhances our capability to study nanocrystal-based devices in *operando* conditions, leading to a deeper understanding that can inform better design and performance improvements.

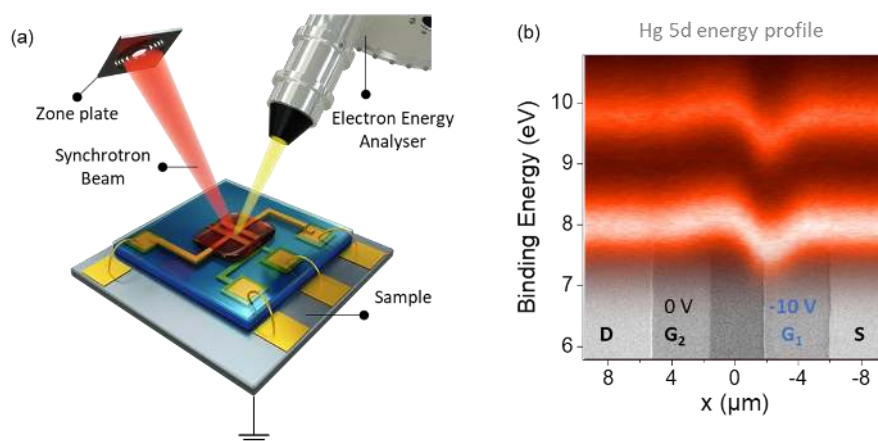


Fig. 1. (a) Schematic of the X-ray photoemission microscope. A soft X-ray beam from the synchrotron is focused on the sample with sub  $\mu\text{m}$  resolution thanks to the zone plate. The photoemission signal is acquired point by point in a scanning mode with a hemispherical electron analyser. (b) Example of *operando* measurements showing a profile of the binding energy of the Hg 5d states over the channel of the FET while gate bias is applied, in the background we report a scanning electron microscopy image of the device to highlight the location of the channel area, where D = drain, S= source and G<sub>1</sub> and G<sub>2</sub> are the gates.

- [1] Gréboval, C. *et al. Chem. Rev.* 121, 3627–3700 (2021)
- [2] Cavallo, M. *et al. Adv. Funct. Mater.* 33, 2300846 (2023)
- [3] Cavallo, M. *et al. Nano Lett.* 23, 1363–1370 (2023)
- [4] Cavallo, M. *et al. Nanoscale* 15, 9440–9448 (2023)
- [5] Khalili, A. *et al. ACS Appl. Electron. Mater.* 5, 4377–4384 (2023)

## Opportunities for the study of surfaces and interfaces in soft condensed matter at the SIRIUS beamline of Synchrotron SOLEIL

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The SIRIUS beamline of the Synchrotron SOLEIL is dedicated to X-ray scattering and spectroscopy of surfaces and interfaces, covering the tender to mid-hard X-ray range (1.1-13 keV) [1,2]. The beamline has hosted a wide range of experiments in the field of soft interfaces and beyond, providing various grazing incidence techniques such as diffraction and wide angle scattering (GIXD/GIWAXS), small angle scattering (GISAXS) and X-ray fluorescence in total reflection (TXRF). Systems studied belong to various fields of interfacial science, and encompass organic layers, block copolymers, MOFs, graphene oxide, solar cells ... SIRIUS also offers specific sample environments tailored for *in situ* complementary experiments on solid [3] and liquid surfaces. Recently, the beamline has added compound refractive lenses associated with a translocator, allowing for the X-ray beam to be focused down to  $10 \times 10 \mu\text{m}^2$  while maintaining a reasonable flux on the sample. We have also equipped our Langmuir trough with a UV-visible spectrometer, to extend the range of *in situ* measurements complementing the X-ray acquisitions.

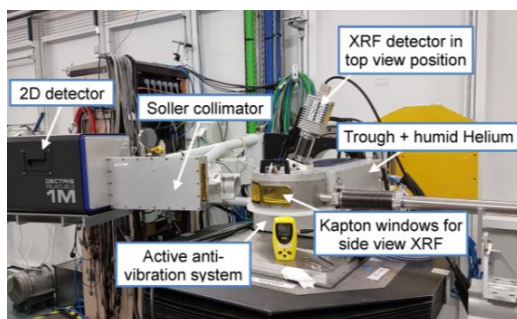


Fig. 1. Langmuir trough for experiments at the liquid-air interface mounted on the 6-axis tower of the multipurpose diffractometer, enabling combined GIXD and XRF measurements.

[1] P. Fontaine, G. Ciatto, N. Aubert and M. Goldmann, *Science of Advanced Materials* **6**, 2312–2316 (2014).

[2] A. Hemmerle, N. Aubert, T. Moreno, P. Kékicheff, B. Heinrich, S. Spagnoli, M. Goldmann, G. Ciatto and P. Fontaine, *accepted in Journal of Synchrotron Radiation* (2023).

[3] M. Galerne, B. Heinrich, A. Hemmerle, P. Fontaine, N. Giuseppone and P. Kékicheff, *ACS Appl. Polym. Mater.* **3**, 661-670, (2021).

# Absolute surface and interface energy analysis of III-V/Si and its consequences on wetting characteristics

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Integration of III-V semiconductors on Si (001) substrates is of great interest for photonic, electronic, and energy harvesting devices.<sup>[1-3]</sup> In this study, we show how the atomic arrangement of the III-V/Si interface affects the system's wetting characteristics. Using density functional theory, we first demonstrate how it is possible to investigate the variations of the absolute interface energy with the chemical potential in heterogeneous materials systems. Especially, we show that charge compensated III-V/Si interfaces are remarkably stable over a large range of chemical potential in agreement with the Electron counting model.<sup>[4,5]</sup> Although it is anticipated that stable compensated III-V/Si interfaces would normally favor complete wetting conditions, it is found that this can be easily balanced by the substrate's initial passivation, which favors in turn partial wetting conditions. Finally, we highlight how surface passivation is crucial in wetting property investigations during heterogeneous epitaxy.

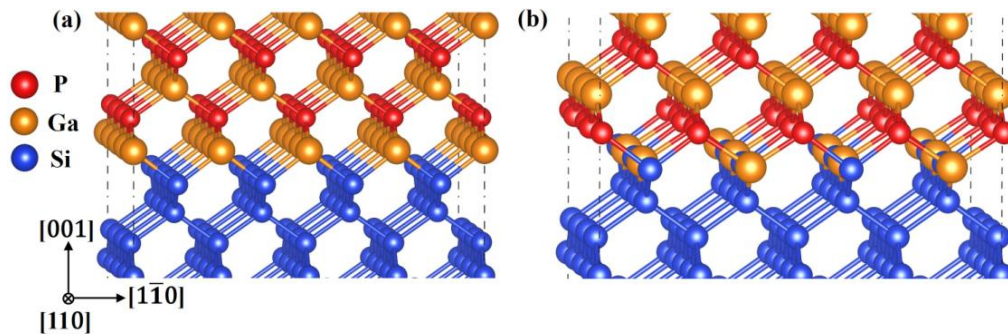


Fig.1. Zoomed atomic configurations: a) Si-Ga abrupt interface, and b) Ga compensated interface (0.5Si: 0.5Ga-P).

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[1] I. Lucci, S. Charbonnier, L. Pedesseau, M. Vallet, L. Cerutti, J.-B. Rodriguez, E. Tournié, R. Bernard, A. Létoublon, N. Bertru, A. Le Corre, S. Rennesson, F. Semond, G. Patriarche, L. Largeau, P. Turban, A. Ponchet, and C. Cornet, *Phys. Rev. Materials* **2**(6), 060401 (2018).

[2] I. Lucci, S. Charbonnier, M. Vallet, P. Turban, Y. Léger, T. Rohel, N. Bertru, A. Létoublon, J. Rodriguez, L. Cerutti, E. Tournié, A. Ponchet, G. Patriarche, L. Pedesseau, and C. Cornet, *Adv Funct Materials* **28**(30), 1801585 (2018).

[3] C. Cornet, S. Charbonnier, I. Lucci, L. Chen, A. Létoublon, A. Alvarez, K. Tavernier, T. Rohel, R. Bernard, J.-B. Rodriguez, L. Cerutti, E. Tournié, Y. Léger, M. Bahri, G. Patriarche, L. Largeau, A. Ponchet, P. Turban, and N. Bertru, *Phys. Rev. Materials* **4**(5), 053401 (2020).

[4] O. Supplie, S. Brückner, O. Romanyuk, H. Döscher, C. Höhn, M. M. May, P. Kleinschmidt, F. Grosse, and T. Hannappel, *Phys. Rev. B* **90**, 235301 (2014).

[5] S. Pallikkara Chandrasekharan, I. Lucci, D. Gupta, C. Cornet, and L. Pedesseau, *Phys. Rev. B* **108**(7), 075305 (2023).

## Collage direct appliqué à la microélectronique : le cas des polymères

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Le collage direct consiste en l'adhésion spontanée de deux surfaces solides sans intermédiaire liquide. Le collage direct de substrats à base de silicium est utilisé et bien connu notamment en microélectronique, par exemple pour la production de substrats de type SOI (silicon-on-insulator). Des critères doivent être strictement respectés afin de pouvoir réaliser un collage direct. La surface doit être suffisamment plane, dépourvue de particules et avoir une microrugosité de surface inférieure à 0,5 nm RMS (Root Mean Square) dans le cas d'un collage direct de silicium hydrophile [1].

Dans cette étude, nous nous focaliserons sur le collage direct avec des films fins de polymère. Notre étude est innovante car les polymères sont des matériaux aux propriétés bien différentes du silicium. En effet, les polymères sont peu ou pas cristallins, beaucoup moins rigides et souvent hydrophobes. Différents films de polymères ont été utilisés pour cette étude : LOR2A, BARC AR26N, SOC HM8102, TOK TDMR et LTC9310. Leur épaisseur est comprise entre 32 nm et 6  $\mu\text{m}$ . Ces polymères ont été déposés sur des substrats de silicium de 200 ou 300 mm de diamètre.

Dans un premier temps, les polymères ont été caractérisés par spectroscopie infrarouge à transformée de Fourier (FTIR), par ellipsométrie et par analyse thermogravimétrique (ATG). Les angles de contact à l'eau de ces polymères sont compris entre 58° et 77°, ce qui est caractéristique de surfaces hydrophobes. À titre de comparaison, l'angle de contact est inférieur à 5° dans le cas du silicium hydrophile ( $\text{SiO}_2$ ) et est égal à 78° pour le silicium hydrophobe passivé (Si). La rugosité de surface de nos polymères mesurée par microscopie à force atomique (AFM) est comprise entre 0,3 et 0,4 nm RMS. Le collage direct est possible entre les films de polymères et les surfaces de silicium hydrophiles et hydrophobes. Les énergies d'adhésion sont comprises entre 40 et 70  $\text{mJ/m}^2$  et les vitesses d'onde de collage entre 10 et 19 mm/s. À angles de contact équivalents, les collages directs avec polymère présentent des énergies d'adhésion et des vitesses d'onde supérieures aux collages directs sans polymère. Les images acoustiques ainsi que les énergies d'adhérence mesurées par la technique du DCB (Double Cantilever Beam) [2] des collages avec BARC sont présentées en **Figure 1**. L'énergie d'adhérence augmente avec la température grâce à l'augmentation de la densité des liaisons covalentes pendant le recuit. Des collages directs sur des substrats rugueux avec nos polymères ont été réalisés et montrent que la limite de collage est étendue en terme de rugosités avec les polymères. Des mesures de réflectivité des rayons X (XRR) ont été réalisées afin d'étudier la fermeture de l'interface de collage.

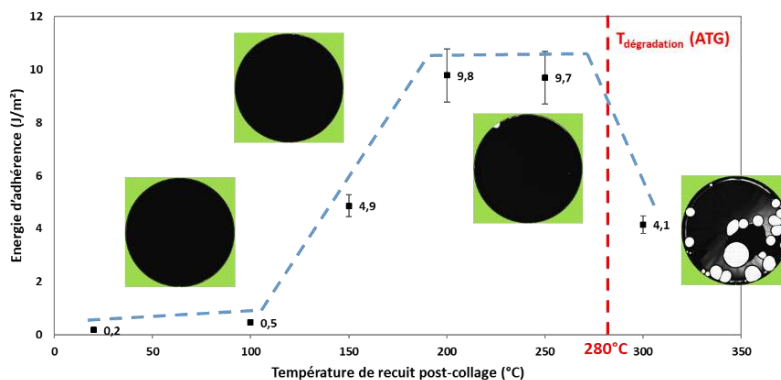


Fig. 1. Énergie d'adhérence en fonction de la température de recuit des collages directs BARC/ $\text{SiO}_2$

[1] H. Moriceau et al., Adv. Nat. Sci. Nanosci. Nanotechnol., 1, 043004 (2011).

[2] W. P. Maszara et al., J. Appl. Phys., 64, 4943 (1988).



## Stable Fluorine Superstructures on Cu(001) and Cu(111)

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The interaction of single fluorine atoms with the copper surface is very poorly studied in comparison with other halogens [1]. Meantime, the copper-fluorine surface interaction is interesting for further investigation and development of Fluorine-ion batteries, for example, on the base of Cu/LaF<sub>3</sub> system [2]. Additional interesting problem is a possible existence of surface copper(I) fluoride recognized as unstable and not isolable in bulk. Indeed, CuF in 3D case readily transforms into CuF<sub>2</sub> and Cu, because of exothermicity of its disproportionation reaction [3]. The lack of detailed experimental studies of metal surface fluorination with low fluorine coverage is partially caused by difficulties to work with reactive fluorine-containing gases and to dose a low concentration of fluorine atoms on the surface. We use the fluorinated fullerene molecule C<sub>60</sub>F<sub>18</sub> at submonolayer coverage as a precursor of F-induced surface structures on Cu crystal surfaces [4]. The F-induced structures on Cu (001) and (111) planes are studied by scanning tunneling microscopy (STM), X-ray photoelectron spectroscopy (XPS) and first-principles calculations based on density functional theory (DFT). The stable superstructures with (2√2×√2)R45-3F cell on Cu(001) and Kagome structures with p(5×5)-12F and p(7×7)-24F periodicity on Cu(111) are observed by STM, see Fig.1. The XPS analysis clearly indicates a strong chemisorption of fluorine atom and Cu(I) oxidation state on the surface. Comprehensive DFT calculations of F adsorption show strong interaction and low diffusion barriers on both surfaces. From the present DFT results the model of (2√2×√2)R45-3F on Cu(001) is proposed and fits well the observed STM contrast [5]. DFT confirms the existence of p(5×5)-12F and p(7×7)-24F superstructures for F/Cu(111), but predicts distortions of the Kagome lattice which are not observed in STM. The stability of the structures is analyzed in terms of the adsorption energy landscape and the F-F interaction.

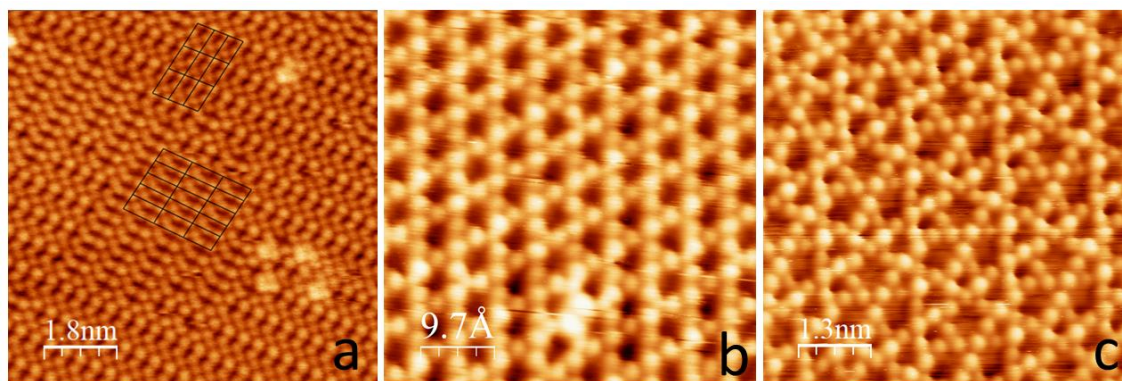


Fig. 1. STM images (a) (2√2×√2)R45° on Cu(001); (b) p(5×5) and (c) p(7×7) on Cu(111).

[1] Andryushechkin *et al.*, *Surf. Sci. Rep.*, **73**, 83 (2018).

[2] Nakano *et al.*, *Chem. Mater.*, **33**, 459 (2021).

[3] Walsh, *et al.*, *Chem. Sci.*, **3**, 2565 (2012).

[4] Oreshkin *et al.*, *J. Phys. Chem. C*, **122**, 24454 (2018).

[5] Petukhov *et al.*, *J. Phys. Chem. C*, **126**, 21390 (2022).

# Synchrotron-based electronic characterization of organic thin films for non-fullerene acceptor solar cells

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The transition from fullerene to non-fullerene acceptors (NFAs) has increased the power conversion efficiency (PCE) of organic photovoltaics (OPV) drastically, reaching PCEs above 19% [1]. As opposed to fullerene acceptors, NFAs have tuneable energy levels, stronger absorption across the solar spectrum, and better thermal stability. The PM6/Y7 polymer donor/NFA binary blend is one of the most promising systems [2] thanks to its broad absorption range, which favors high photocurrents in such based devices [3]. One of the crucial factors that determines the final efficiency of the device concerns the band alignment of the frontier orbitals. This point has not been explored until now in the blend system PM6/Y7, in particular by varying the ratio between the donor and acceptor molecule.

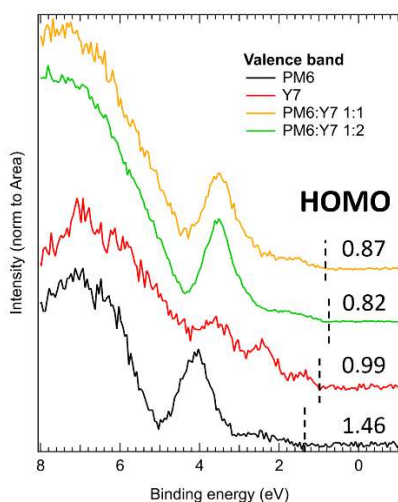


Figure 1. Valence band spectra of the neat PM6 and Y7 thin films and the blend PM6:Y7 with different

characteristic Y7 valence band's shape, we noticed a strong modification of the Cl 2p core level shape as a function of the thickness of the sprayed film, which is highlighted by the appearance of a new feature.

In conclusion, through the observation of significant changes in the electronic structure and frontier orbitals between the pure molecules and the blend, along with the emergence of a new feature in the Cl 2p core level at the interface between the NFA and ETL, we have taken a significant step forward in understanding this highly efficient unexplored system.

[1] L. Zhu, et al., Nature Materials 21, 656 (2022)

[2] Y. Cui et al. Nat Commun 10, 2515 (2019)

[3] R. Yu et al., J. Energy Chem. 61, 29 (2021)



# Scanning Tunneling Microscope as a characterization tool for single atom catalysis ? Experimental observations and simulation results

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Single atom catalysts (SAC) have attracted much interest since the last decade. This domain is particularly important in the context of climate change and the necessity to reduce drastically the fossil energy consumption and rare resources employment. However, in spite of important quantity of results already obtained, a real breakthrough in the discovery of effective catalysts is still uncertain. The major bottleneck to optimize the efficiency and the stability of SACs is the lack of understanding about the reaction mechanism of these systems at the atomic scale. Among the available techniques, the scanning tunneling microscope (STM) associated with density functional theory (DFT) calculations could be an interesting means to characterize some model systems [1].

In this work, we present our STM observations and DFT results of two single atoms (Au and Co) evaporated on self-assembled 2D domains of terephthalic acid (TPA) on Ag(001) substrate [2]. By comparing the different behaviors of these 2 single atoms, we have identified that the different contrast of Au atoms originates from its adsorption site and the attachment of diffusing H atoms from the surrounding defects in TPA layer [3]. The reactivity of single Au atom towards the H atoms could eventually explain the desorption of Au adatoms.

The behavior of Co single atom is much simple. Explained by a significant adsorption energy calculated by DFT, Co atom is firmly bounded to the TPA by sitting on top of the center of the benzene ring. In spite of this strong attachment, these single Co atoms are also sensitive to the surrounding H atoms. To illustrate this, the reaction paths of a model system using Co atom as SAC are predicted and simulated STM images of the associated intermediate states are presented.

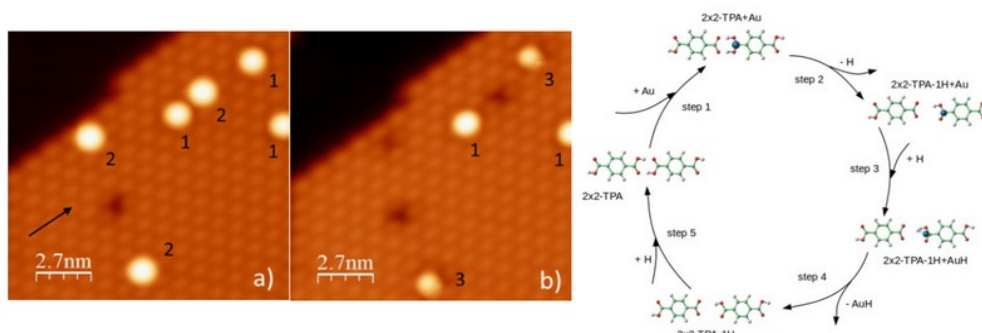


Fig.1. STM images of Au adatoms before and after modification and a proposed Au atom desorption mechanism,

[1] A. J. Therrien, A. J. R. Hensley, M. D. Marcinkowski, R. Zhang, F. R. Lucci, B. Coughlin, A. S. Schilling, J.-S. McEwen, E. C. H. Sykes, *Nature Catalysis* 1 (2018) 192–198.

[2] H. Tang, C. Durand, R. Coratger, *Surfaces and Interfaces* 25 (2021) 101170.

[3] J. Heintz, C. Durand, H. Tang, R. Coratger, *Phys. Chem. Chem. Phys.* 22 (6) (2020) 3173–3183

# Molecular structure of Langmuir-Blodgett monolayer probed by conventional and phase-sensitive sum frequency generation vibrational spectroscopy.

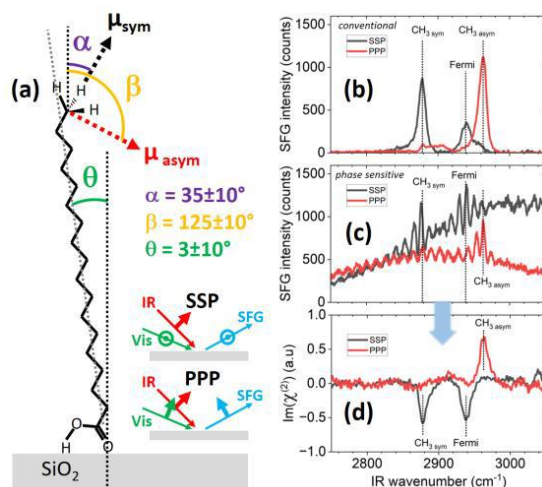
## Titre en français : Structure moléculaire de monocouches de Langmuir-Blodgett sondée par spectroscopie vibrationnelle de génération de fréquence somme conventionnelle et sensible à la phase

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Langmuir-Blodgett (LB) monolayers constitute a fundamental object of molecular physics, which finds practical applications in various fields: electronics [1], optics, applied chemistry, micromechanics, biology and medicine [2] etc. In this study, fatty acids ( $H_3C-(CH_2)_{n-2}-COOH$ ) and fatty alcohols ( $H_3C-(CH_2)_{n-1}-OH$ ) deposited on glass substrates are used as model objects. The vibrational modes of methylene  $CH_2$  and methyl  $CH_3$  groups probed by Sum-Frequency Generation (SFG) [3] and by Phase-Sensitive SFG (PS-SFG) [4] vibrational spectroscopies provide detailed information on the structure and conformation of the ordered two-dimensional molecular layer. Here, using conventional SFG and PS-SFG, we determine the orientation of the  $CH_3$  terminal methyl group and by extension the angle of inclination (tilt) of the alkyl chain in the all-trans conformation of a monolayer of oleic acid ( $H_3C-(CH_2)_{16}-COOH$ ) on glass lead (see figure). The sensitivity of the PS-SFG technique to the molecular absolute orientation inside films opens the route to the understanding of biological interfaces [5]. In this topic, the ultimate objective concerns confined water and the access to its orientation inside peptide multilayers and its ability to control the functionality of biomolecules [6].



Langmuir-Blodgett monolayer of oleic acid ( $H_3C-(CH_2)_{16}-COOH$ ) on glass: (a) Structure and orientation of the chain deduced by conventional SFG and PS-SFG. Schematic diagram of the ssp and ppp polarization combinations for the three beams concerning the SFG. (b) Spectra of conventional SFG in ssp (black) and ppp (red). (c) SFG interferograms with GaAs in ssp (black) and ppp (red). Imaginary part of the second order non-linear susceptibility  $Im\{\chi_{H_3C-(CH_2)_{16}-COOH}^{(2)}\}$ . The sign of this parameter is directly linked to the orientation of the vibrational modes. It is extracted from PS-SFG spectra by inverse Fourier transform followed by temporal filtering and finally by Fourier transform.

- (1) Mandeep Singh, Navpreet Kaur and Elisabetta Comini, J. Mater. Chem. C **8**, 3938 (2020)
- (2) Debasis Samanta and Amitabha Sarkar, Chem. Soc. Rev. **40**, 2567–2592 (2011)
- (3) Z. Guo, W. Zheng, H. Hamoudi, C. Dablemont, V.A. Esaulov, B. Bourguignon, Surf. Sci. **602**, 355 (2008)
- (4) V. Ostroverkhov, G. A. Waychunas, and Y. R. Shen, Phys. Rev. Lett. **94**, 046102 (2005)
- (5) M. Gabaji, J. Médard, A. Hemmerle, J. Pinson and J. P. Michel, Langmuir **36**, 2534 (2020)

(6) Tetiana Mukhina et al. J.Phys.Chem.Lett. **10**, 7195 (2019)

## Near Ambient Pressure-X-ray Photoelectron Spectroscopy study of GaAs based photoelectrodes

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Among III-V semiconductor materials, GaAs is a promising candidate for high performance photocatalysis owing to its appropriate band edge energies and its transport properties. Since photoelectrochemical (PEC) processes take place in aqueous electrolyte, understanding the nature of water interactions with semiconductor surface is of great interest. Moreover identifying the oxidation and reduction reactions taking place at the photoelectrode/electrolyte interface is a major objective, instability against corrosion for PEC applications being one significant limitation of GaAs photoanode while GaAs photocathodes are stable.

In order to understand the water/GaAs interface chemistry under realistic conditions, we have investigated the interfacial interactions using Near-Ambient Pressure X-ray Photoelectron Spectroscopy (NAP-XPS). Experiments were carried out at room temperature under water exposure and combined water exposure and red-laser (671 nm) illumination. Pressure in the spectrometer analysis chamber was 2 mbar under a continuous-flow mode. Two types of photocathodes were investigated: Zn-doped ( $10^{16}\text{cm}^{-3}$ ) *p*-type to GaAs wafer and 1  $\mu\text{m}$ -thick molecular beam epitaxy (MBE) grown GaAs layer on *p*-Si substrates. Native oxides were not altered through cleaning procedures prior to XPS measurements in order to investigate semiconductor based photoelectrodes in real conditions. Consequently, water molecules interacted mostly with GaAs oxide surface. We found that water interactions with GaAs electrodes were highly related to the morphology and composition of the oxides present at the different GaAs surfaces.

This research is supported by the “France 2030” French National Research Agency NAUTILUS Project (Grant no. ANR-22-PEHY-0013).

## **NMR Relaxation study of the organization of the interfacial layer in presence and absence of solvent of the interface Polymers/Silica**

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In order to modify the interaction between solid and the surrounding medium one of the ways is to graft polymers at the interface. The interfacial layer can act as a coupling agent a screening factor and enhance properties of the interface [1]. Polymers chains grafted into solid surfaces are fundamental in many applications in colloid and surface science, as well as in biology

The  $^1\text{H}$  and  $^{13}\text{C}$  NMR technique is used to study the behavior of the poly(ethylene oxide) (PEO) chains grafted chemically on silica in presence or not of solvent. One of the main objectives of this work is to determine the disposition of monomer units near the surface and their concentration

A noticeable influence of the different physicochemical parameters on the conformation of the grafted macromolecules is evinced. Different models are proposed for different length of the grafted polymer chains on the surface. in absence and in presence solvent. Without solvent, the macromolecules lie very flat and the layer is more organized. In the presence of solvent, the chains spread out and adopt a more extended conformation and the local concentration of monomers decreases [2].

[1] T. Tajouri, M.A.Ben Mariem and H. Hommel, *Concepts Magn. Reson.* 44, 306 (2015).

[2] T. Tajouri, *Ann Adv Chem.* 6, 60 (2022).

## Tuning Electronic Properties in Nanoparticles of Gold

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Nanoparticles (NPs) have attracted a lot of attention in many fields of research (e.g., chemistry, biology, material and environmental sciences) in recent years [1]. Depending on their size, geometrical shape and composition, NPs can have various applications and can be synthesized by different methods. One of these methods is pulsed laser ablation in liquid (PLAL) which can be used to produce NPs of any kind of material including metals, alloys and semiconductors [2]. The PLAL synthesized nanoparticles are charged and free of surfactants, thus their colloids are very stable and pure. PLAL NPs have showed a great potential as plasmonic photosensitizers [3]. In photovoltaic systems, heterojunctions containing plasmonic materials are considered to expand the light absorption spectrum of semiconductors (SC) by excitation of plasmon waves [4]. By selecting the proper material and size, it is possible to tune the plasmon resonance of NPs, which can result in a photocurrent that is no longer constrained by the semiconductor band gap.

The aim is to improve the injection efficiency of the NP/semiconductor interface taking advantage of PLAL NPs in which stable colloids can be produced without the presence of surfactant molecules. To control the Schottky barrier height (SBH) at the metallic NP/SC interface [5], it is necessary to take into account the interface states that deviate the Schottky barrier from the expected Schottky-Mott rule behavior [6]. We expect to tune SBH up and down with high flexibility by using halogen-based interlayers [7].

We first studied an interlayer composed of either NaBr or NaI halide to understand its influence on the metallic substrate. The surface of a gold single crystal is progressively covered in situ with halide layer using an effusion cell. The corresponding coverage is evaluated by XPS and, UPS is used for work function measurements. We observed that as we increase the coverage, the work function of the metal decreases. Secondly, to produce high quality heterojunctions from colloidal solutions of PLAL Au NPs and avoiding aggregation as much as possible, an electrospray was used to deposit NPs under UHV on a TiO<sub>2</sub> crystal directly from the NP stock solution. After electrospray deposition of the NPs, the heterojunction was characterized by XPS. Ambient AFM measurement was performed at the microscopic level to study the homogeneity of the deposition as well as possible NP aggregation.

[1] V. Amendola *et al.*, J. Phys.: Condens. Matter, 29, 203002 (2017)

[2] D. Amans *et al.*, Applied Surface Science, 488, 445-454(2019)

[3] H. Tang *et al.*, J. Chem. Phys. 152, 220901 (2020)

[4] D. C. Ratchford *et al.*, Nano Letters, 17, 6047 (2017)

[5] Z. Sun and *et al.*, Sci. Rep. 11, 338 (2021).

[6] R. T. Tung *et al.*, Appl. Phys. Rev. 1, 011304 (2014)

[7] B. E. Coss *et al.*, Appl. Phys. Lett. 95, 222105 (2009)

# Leveraging Bayesian Optimization to Enhance Convergence in Bulk and Surface Simulations: A Focus on Charge Mixing Parameters in DFT

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## Abstract:

Density Functional Theory (DFT) has been a cornerstone theory in materials science and nanotechnology for simulating material properties, providing invaluable insights. However, the computational demands associated with surface simulations, especially for complex surfaces, pose significant challenges [1]. A crucial bottleneck in DFT simulations is the iterative self-consistent update of electronic charge density, known as "charge mixing," resulting in substantial computational energy overhead. To address these challenges, we turn to Bayesian optimization, a machine learning technique tailored to explore parameter spaces efficiently, thus finding optimal solutions [2].

Our research aims to boost the efficiency of DFT calculations and reduce computational energy consumption by fine-tuning the charge mixing process using Bayesian optimization. This approach not only expedites the convergence of bulk simulations but also the convergence of surface simulations. To demonstrate the real-world impact of Bayesian optimization-driven charge mixing optimization, we conducted experiments on two materials: Silicon Carbide (SiC) and Gallium Cobalt (GaCo). We optimized charge parameters for these bulk materials, witnessing a remarkable reduction in required iterations for convergence, down to 14 for SiC and 9 for GaCo, compared to 20 for SiC and 14 for GaCo (Table 1). These optimized parameters were then applied to simulate interfaces of both materials, exploring the 001 and 111 surfaces. Our results, as detailed in Table 1, underscore noticeable improvements in convergence and therefore the computational efficiency achieved through Bayesian optimization-driven charge mixing parameters optimization.

In conclusion, our research highlights the pivotal role of Bayesian optimization in advancing the convergence of materials science simulations. Through the optimization of charge mixing parameters, we have significantly alleviated computational burdens and achieved more efficient and cost-effective bulk and surface simulations.

**Table 1:** Optimized charge mixing parameters for GaCo and SiC.

Material	AMIN	AMIX	BMIX	NELMDL
GaCo	0.1636	0.3492	1.4459	-2
SiC	0.6118	0.9217	1.9961	-2

**Table 2:** Iteration counts for GaCo and SiC bulk, and surface structures.

Material	GaCo (bulk)	GaCo (001)	GaCo (111)	SiC (bulk)	SiC (001)	SiC (111)
Standard	13	27	26	14	23	32
Optimized	9	21	20	10	20	36



**References**

- [1] D.S. Sholl, J.A. Steckel, Density Functional Theory: A Practical Introduction, Wiley, Hoboken, N.J, 2009.
- [2] J. Bergstra, R. Bardenet, Y. Bengio, B. Kégl, in: J. Shawe-Taylor, R. Zemel, P. Bartlett, F. Pereira, K.Q. Weinberger (Eds.), Adv. Neural Inf. Process. Syst., Curran Associates, Inc., 2011.

# Unravelling the charge distribution at electrochemical interfaces using in situ surface resonant X-ray diffraction

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Electro-catalysts make it possible to accelerate electrochemical reactions, with important applications in several fields, such as energy storage, chemical synthesis, biosensors, water electrolysis.

The electro-catalytic activity is largely influenced by the charge distribution at the electrochemical interface, the few Ångstrom thick metal-liquid interface region where the exchange of charges takes place. Understanding the involved mechanisms is of paramount importance. It is above all a question of being able to characterize the structural and electronic properties of the catalyst surface and of the charge distribution in the solution. Nevertheless, unlike for the atomic structure characterization, there is currently no experimental method to specifically probe the electronic structure at this interface.

We present here a new approach, which allows the direct experimental measurement of the charge distribution at the electrochemical interface. This was achieved by combining experimental and theoretical approaches, i.e. coupling *in situ* experiments of Surface Resonance X-Ray Diffraction (SRXRD) with first-principle simulation of the measured spectra. FDMNES code, recently extended for the simulation of surface resonant diffraction experiments [1], has now been developed for the electrochemical interface description, to consider the presence of the electrolyte facing the crystal and the effect of the applied external electric field.

We succeeded here in measuring for the first time the spatial charge distribution at the electrochemical interface of the archetypal system Pt(111) in acidic solution, for which the surface charge influence on common electrochemical reactions is well known (see figure 1).

Our work has proven that *in situ* SRXRD coupled with *ab initio* calculations provides a new tool that gives access to the surface electronic charge distribution of electrochemical interfaces [2,3]. This method will make a valuable contribution to the up to now lacking experimental evidence of surface charge distribution, a challenging topic for the understanding of the electrochemical reactivity and to validate the theoretical predictions.

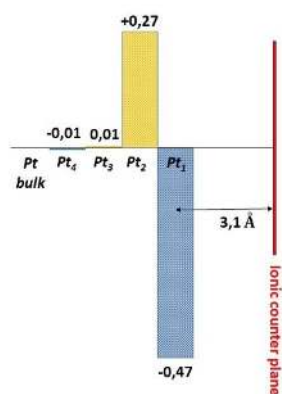


Fig. 1. Schematic representation of the charge distribution, charge per platinum atom, at the electrochemical interface of the Pt(111) crystal in 0.1M H<sub>2</sub>SO<sub>4</sub> at 350 mV<sub>RHE</sub>.

[1] Y. Joly et al. J. Chem. Theory Comput. 2018, 14( 2), 461

[2] Y. Soldo-Olivier, E. Sibert, M. De Santis, Y. Joly, Y. Gründer. ACS Catalysis 2022, 12, 2375

[3] Y. Grunder, C. A. Lucas, P. Thompson, Y. Joly, Y. Soldo-Olivier J. Phys. Chem. C 2022, 126 (9), 4612