JSI2025 : Journées Surfaces et Interfaces 2025 (JSI)

29-31 janvier 2025 - Orsay (France)

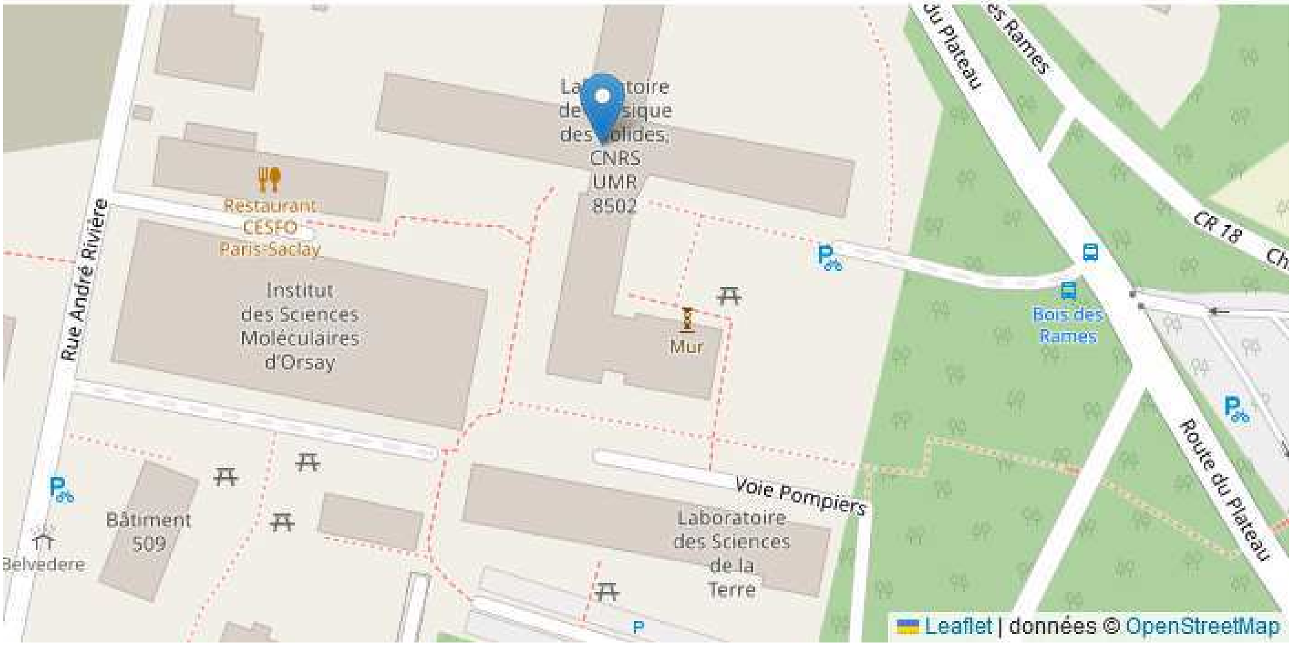
Programme

Lieux

Institut des Sciences Moléculaires d'Orsay (ISMO) : accueil et déjeuners
Laboratoire de Physique des Solides (LPS) : présentations, session poster et exposants, pause-café

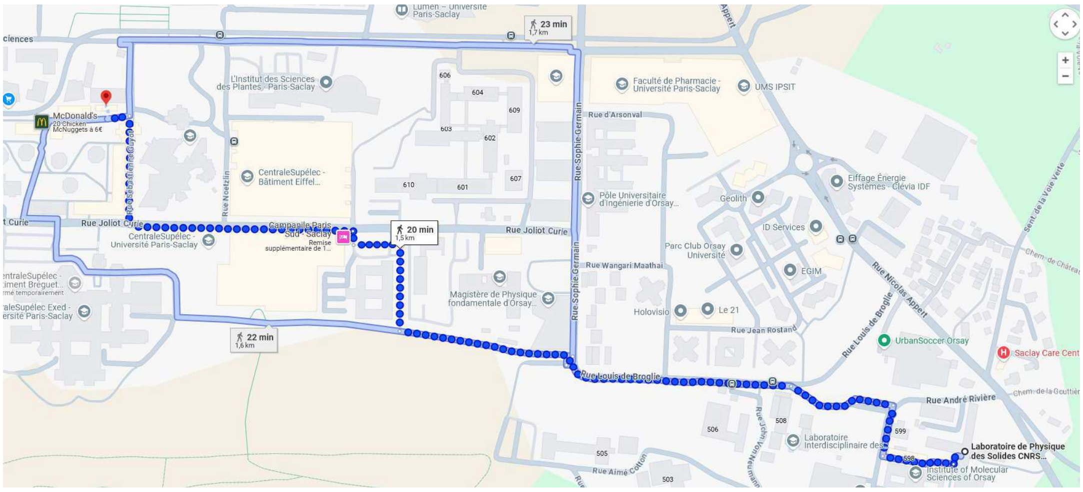
Option 1 : Par le RER B, direction Saint-Rémy les Chevreuse, station "Massy-Palaiseau" puis emprunter la ligne de bus 91-06 (en direction du Christ de Saclay) ou la ligne de bus express 91.10 (en direction de St Quentin en Yvelines – Montigny Le Bretonneux) jusqu'à l'arrêt "Université Paris-Saclay, Orsay" – Rejoindre le LPS à pied, 10 minutes, à plat.

Option 2 : Par le RER B, direction Saint-Rémy les Chevreuse, descendre à la station "Orsay Ville" puis emprunter la ligne de bus 7 (en direction du Plateau de Moulon - Corbeville) jusqu'à l'arrêt "Bois des rames". Le LPS est le bâtiment juste en face de l'arrêt de bus.



Diner de Gala – jeudi 30 janvier 2025 – 19h30

Brass & Co, 24 - 26 Mail Pierre Potier, 91190 Gif-sur-Yvette
Arrêt Joliot Curie bus 91-06 ou 91-08 ou EXP91-10



Oratrices invitées / Orateurs invités

- **Grégory ABADIAS**, Pprime (Poitiers), *Comment piloter la morphologie de couches métalliques ultra-minces ? Apport des mesures in situ et en temps réel durant et après la croissance*

- **Caroline BORDERON**, IETR (Nantes), *Matériaux ferroélectriques et antiferroélectriques : propriétés diélectriques et applications*

- **Olivier BOULLE**, Spintec (Grenoble), *Electrical manipulation and detection of magnetic skyrmions for memory and logic applications*

- **Fabian CADIZ**, Laboratoire de Physique de la Matière Condensée (Palaiseau), *Optical spectroscopy of excitons in 2D semiconductors*

- **Thomas CORNELIUS**, IM2NP (Marseille), *Ferroelectric materials in the light of synchrotron X-ray diffraction*

- **Jean-François DAYEN**, IPCMS (Strasbourg), *Opto-electric control of van der Waals ferroelectric heterostructures : opportunities for beyond-Moore applications*

- **Giorgia FUGALLO**, Laboratoire de Physique de l'ENS (Paris), *From 3D to 2D materials: emergent phenomena in the electronic phononic and thermal response*

- **Anne HEMERYCK**, LAAS (Toulouse)*, Structure et Propriétés des Interfaces Semiconductrices : Une approche atomistique et multi-échelle*

- **Geoffroy KREMER**, IJL (Nancy), *La spectroscopie de photoémission résolue en angle comme outil unique pour l'étude des propriétés électroniques des solides à l'équilibre et hors-équilibre*

- **Anne LAFOSSE**, ISMO (Orsay), *Désorptions non-thermiques de glaces moléculaires : sur la piste des mécanismes*

- **David LOFFREDA**, Laboratoire de Chimie de l'ENS (Lyon), *Ab Initio Models of Functionalized Gold Nanoparticles and Surfaces for Various Applications*

- **Pierre MALLET**, Institut Néel (Grenoble), *Interlayer coupling and twist angle in 2D van der Waals systems : An STM approach*

- **Erwan-Nicolas PAINEAU**, LPS (Orsay), *Structure, molecular confinement and photocatalysis applications in geo-inspired clay nanotubes*

- **Federico PANCIERA,** C2N (Palaiseau)**,** *Real-time observation of III-V nanowire growth by in-situ TEM*

- **Léa-Laetitia PONTANI**, Laboratoire Jean Perrin (Paris), *Biocompatible and biomimetic droplets to probe tissue mechanics*

- **Fausto SIROTTI,** Laboratoire de Physique de la Matière Condensée (Palaiseau)**,** *Spectroscopie des photoélectrons pompe/sonde résolue en temps : la structure électronique pour étudier les transitions de phase.*

- **Konstantinos TERMENTZIDIS,** CETHIL (Lyon), *Thermal transfer through interfaces and close to free surfaces via atomistic simulations*

Mercredi 29 janvier 2025

12:00 - 13:30	Accueil des participant.e.s - Remise des badges – buffet (Hall de l’ISMO)

13:30 - 14:00	Ouverture des JSI (Amphi Blandin - LPS)

Session Propriétés thermiques (Amphi Blandin - LPS) – modération : Aimeric Ouvrard

14:00 - 14:45	*From 3D to 2D materials: emergent phenomena in the electronic phononic and thermal response*, **Giorgia FUGALLO**, Laboratoire de Physique de l'ENS (Paris)
14:45 - 15:30	*Thermal transfer through interfaces and close to free surfaces via atomistic simulations*, **Konstantinos TERMENTZIDIS**, CETHIL (Lyon)

15:30 - 16:00	Pause café (Hall du LPS)

Session Croissance (Amphi Blandin - LPS) – modération : Antonio Tejeda

16:00 - 16:45	*Real-time observation of III-V nanowire growth by in-situ TEM*, **Federico PANCIERA**, C2N (Palaiseau)
16:45 - 17:30	*Comment piloter la morphologie de couches métalliques ultra-minces ? Apport des mesures in situ et en temps réel durant et après la croissance*, **Grégory ABADIAS**, Pprime (Poitiers)
17:30 - 18:15	*Structure et Propriétés des Interfaces Semiconductrices : Une approche atomistique et multi-échelle*, **Anne HEMERYCK**, LAAS (Toulouse)

Jeudi 30 janvier 2025

Session Réactivité (Amphi Blandin - LPS) – modération : Alina Vlad

08:30 - 09:15	*Ab Initio Models of Functionalized Gold Nanoparticles and Surfaces for Various Applications*, **David LOFFREDA**, Laboratoire de Chimie de l'ENS (Lyon)
09:15 - 10:00	*Désorptions non-thermiques de glaces moléculaires : sur la piste des mécanismes,* **Anne LAFOSSE**, ISMO (Orsay)

10:00 - 10:30	Pause café (Hall du LPS)

Session Matière molle (Amphi Blandin - LPS) - modération : Eric Le Moal

10:30 - 11:15	*Biocompatible and biomimetic droplets to probe tissue mechanics*, **Léa-Laetitia PONTANI**, Laboratoire Jean Perrin (Paris)
11:15 - 12:00	*Structure, molecular confinement and photocatalysis applications in geo-inspired clay nanotubes,* **Erwan-Nicolas PAINEAU**, LPS (Orsay)

12:00 - 13:30	Déjeuner (Hall de l'ISMO)

Session Magnétisme (Amphi Blandin - LPS) - modération : Stanislas Rohart

13:30 - 14:15	*Electrical manipulation and detection of magnetic skyrmions for memory and logic applications*, **Olivier BOULLE**, Spintec (Grenoble)

Session Matériaux ferroélectriques (Amphi Blandin - LPS) – modération : Sylvia Matzen

14:15 - 15:00	*Matériaux ferroélectriques et antiferroélectriques : propriétés diélectriques et applications*, **Caroline BORDERON**, IETR (Nantes)

Session Exposants (Amphi Blandin - LPS)

15:00 - 15:30	Présentation flash des exposants (Amphi Blandin - LPS)

15:30 - 17:00	Session Poster - Pause café (Hall du LPS)

Session Matériaux ferroélectriques (Amphi Blandin - LPS) – modération : Sylvia Matzen

17:00 - 17:45	*Ferroelectric materials in the light of synchrotron X-ray diffraction,* **Thomas CORNELIUS**, IM2NP (Marseille)
17:45 - 18:30	*Opto-electric control of van der Waals ferroelectric heterostructures : opportunities for beyond-Moore applications,* **Jean-François DAYEN**, IPCMS (Strasbourg)

19:30 - 23:00	Diner de gala (Brass & Co) pour les inscrit.e.s

Vendredi 31 janvier 2025

Session Matériaux 2D (Amphi Blandin - LPS) – modération : Julien Chaste

08:30 - 09:15	*Optical spectroscopy of excitons in 2D semiconductors*, **Fabian CADIZ**, LPMC (Palaiseau)
09:15 - 10:00	*Interlayer coupling and twist angle in 2D van der Waals systems : An STM approach*, **Pierre MALLET**, Institut Néel (Grenoble)

10:00 - 10:30	Pause café (Hall du LPS)

Session Photoémission (Amphi Blandin - LPS) – modération : Mylène Sauty

10:30 - 11:15	*Spectroscopie des photoélectrons pompe/sonde résolue en temps : la structure électronique pour étudier les transitions de phase*, **Fausto SIROTTI**, LPMC (Palaiseau)
11:15 - 12:00	*La spectroscopie de photoémission résolue en angle comme outil unique pour l'étude des propriétés électroniques des solides à l'équilibre et hors-équilibre*, **Geoffroy KREMER**, IJL (Nancy)

12:00 - 12:15	Remise des prix du Meilleur Poster Etudiant (Amphi Blandin - LPS)
12:15 - 12:30	Clôture des JSI (Amphi Blandin - LPS)
12:30 - 13:00	Lunchbox (Hall de l'ISMO)

Liste des posters

Session Croissance		
P1 🏅	How AFM and KPFM analysis of Ar etched n-GaN surfaces relates to leakage current measurements in Schottky barrier diodes	Amir Al Abdallah (IEMN, Lille et LERMA, Paris)
P2	Optimization of Crystalline Structures at CIGS/Metal Oxide Interfaces and Analysis of Their Properties for Improved Solar Cell Performance	Hassan Denawi (IMN, Nantes)
P3	1D chains of dye molecules on ultrathin insulators	Eric Le Moal (ISMO, Orsay)
P4	Atomic structure of metallic nanoparticles from EXAFS: transition from monolayer-thick 2D to 3D strained Ag nano-clusters on Al_2O_3(0001)	Rémi Lazzari (INSP, Paris)
P5	Atomic triangulation of the Al_2O_3 layer on a Ni_3Al(111) crystal	Philippe Roncin (ISMO, Orsay)
P6 🏅	Charge transfer between plasmonic PdAg nanoparticles and C60 molecules	Xingtong Li (ISMO, Orsay)
P7 🏅	Croissance et propriétés électroniques des allotropes de phosphorène	Wissem Ghariani (MPQ, Paris)
P8 🏅	Electric-field-assisted phase switching in GaAs nanowires	Qiang Yu (C2N, Palaiseau)
P9	Epitaxial Growth of CaF_2 on Functionalized Si(100) Surfaces: Development of Thin Insulating Layers as a Platform for Nanoscale Device Research	Damien Riedel (ISMO, Orsay)
P10	GIXRD study of epitaxial CuO films grown on $SrTiO_3$(100) by atomic oxygen assisted MBE	Maurizio De Santis (Néel, Grenoble
P11	Grazing Incidence Fast Atom Diffraction in high-pressure conditions	Arindam Mukherjee (ISMO, Orsay et INSP, Paris)
P12 🏅	In-Situ TEM Observation of III-V Nanowire Nucleation on Si substrate	Chen Wei (C2N, Palaiseau)
P13 🏅	Nano-architecture of mixed molecular layers on a silver surface	Yimin Guan (ISMO, Orsay)
P14	Study of Ga for Cd ion exchange under Ga gas precursor	Géraldine Hallais (C2N, Palaiseau)
P15 🏅	Towards single molecule femtoseconde dynamics	Keke Yuan (ISMO, Orsay)
P16 🏅	Ultra-thin films of lead iodide on graphene: influence of the substrate on the opto-structural properties probed in real time	Christian Perest Sonny Tsotezem (ISMO, Orsay)
Session Réactivité		
P17 🏅	Investigation of magnetite oxidation to maghemite via in situ XPS analysis during annealing in dry air	Saida Mtakham (ICB, Dijon)
P18 🏅	Self-Assembled $Ti_3C_2T_X$ MXene Thin Films for High-Performance Ammonia Sensors	Elmehdi Ould Maina (COSYS-IMSE, Marne-la-Vallée et LPCIM, Palaiseau)
Session Matière molle		
P19 🏅	Interfacial self-assembly between polydiacetylene and graphene oxide	Alexia Bistintzanos (INSP, Paris)

P20	Langmuir-Blodgett monolayers: a joint study by femtosecond vibrational spectroscopy and Grazing Incidence X-ray Diffraction	Céline Dablemont (ISMO, Orsay)
P21 🏅	Study and Characterization of TzDA Langmuir Films for Polydiacetylene-Based Sensors	Maria Kandyli (INSP, Paris et LyRIDS, Paris)
Session Magnétisme		
P22	Magnetic skyrmions in ultrathin magnetic films	Stanislas Rohart (LPS, Orsay)
Session Matériaux 2D		
P23	Characterization of the Electrical Properties of 2D Materials via Atomic Force Microscopy	Andrea Cerreta (Park Systems)
P24 🏅	Conception of a new electron microscope for surface science	Florent Vallée (LAC, Orsay)
P25 🏅	Control of large-area 2D crystals-noble metals interaction via interfacial alloying	Hulerich Camel Tchouekem (IPR, Rennes)
P26	Controlling the luminescence of 2D materials using an STM	Eric Le Moal (ISMO, Orsay)
P27	Diffraction of fast heavy noble gas, Ne, Ar, Kr Xe, on a LiF(001) surface	Philippe Roncin (ISMO, Orsay)
P28 🏅	Doping tunable charge density waves in misfit layer compounds	Hugo Le Du (INSP, Paris)
P29 🏅	Electronic control of two-dimensional semiconductor photoluminescence on the nanoscale	Elysé Laurent (ISMO, Orsay)
P30	Electronic Structure Evolution in the Temperature Range of Metal-Insulator Transitions on Sn/Ge(111)	Antonio Tejeda (LPS, Orsay)
P31	Functionalization of silicene by small molecules studied by scanning tunneling microscopy	Geoffroy Prévot (INSP, Paris)
P32 🏅	High performance NO_2 gas sensor at room temperature based on a highly compacted ultra-thin WS2 nanosheets film	Ran Li (LPICM, Palaiseau et COSYS-IMSE, Marne-la-Vallée)
P33 🏅	Optimization of synthesis and growth of layered ferromagnetic oxides for spintronics	Dorian Morley (IPR, Rennes, ISCR, Rennes)
P34	Phase transition in bilayer WSe_2/III-V heterostructure	Meryem Bouaziz (C2N, Palaiseau)
P35	Renforcement de l'adhésion moléculaire pour l'assemblage de verres de silice : rôle de l'activation des surfaces par plasma	Vivien Ménard (CIMAP, Caen)
P36	Self-Trapped Excitons in 2D Hybrid Perovskites	Olivier Plantevin (LPS, Orsay)
Session Photoémission		
P37	Core-level binding energy shifts in ultrathin alkali-halide films on metals	Eric Le Moal (ISMO, Orsay)
P38	Engineering surface band bending in rutile TiO_2 through defect manipulation	Gregory Cabailh (INSP, Paris)
P39 🏅	Etude de répartition du poids spectral en ARPES avec le logiciel chinook	Cynthia Léna Ndjimi (IJL, Nancy)
P40	In situ photoemission spectroscopies to reveal surface transfer doping on hydrogenated milled nanodiamonds	Jean-Charles Arnault (NIMBE-CEA, Gif sur Yvette), Hugues Girard (NIMBE-CEA, Gif sur Yvette)

🏅 Poster étudiant éligible au prix du Meilleur Poster

Résumés des présentations orales

From 3D to 2D materials:
Emergent Phenomena in the Phononic and Thermal Response

Giorgia FUGALLO[1,2]
[1]*Laboratoire de Physique de l'ENS, Département de Physique, École Normale Supérieure, Université PSL, Université PSL, Sorbonne Université, Université Paris Cité, CNRS, 75005 Paris, France*
[2]*European Theoretical Spectroscopy Facility (ETSF)*

*giorgia.fugallo@phys.ens.fr

In many nanostructured materials, while strong covalent bonding provides the stability of the sub-nanometric elementary units, the whole assembly is held together by weak van der Waals interactions. The individual building blocks hence maintain most of their intrinsic characteristics also when arranged together to form a crystalline solid. In principle, novel material properties can be thus tailored by controlling those of the elementary units. The bottom-up synthesis strategy for new materials has been actively pursued since the '80s, gaining significant attention with the exploration of small atomic aggregates, nanoclusters, fullerenes, nanotubes, and more [1-2].

In this context, the interest in low-dimensional materials is self-evident. On the one hand, the physics of many-body systems, limited in 2D or 1D, unveils a plethora of unusually fascinating properties. Simultaneously, the reduction of dimensionality enables gedanken experiments for testing and enhancing our understanding of physical models.

In this presentation, I will discuss how both the lattice and thermal responses change with decreasing dimensionality, elucidating the factors contributing, for example, to the breakdown of the Fourier law for thermal conductivity, the emergence of some exotic phenomena, such as the possibility to observe heat-wave propagation (second sound) at room temperature and the superradiance of optical phonons during the 2D → 3D crossover [3-8].

[1] M. S. Dresselhaus et al, *Science of Fullerenes and Carbon Nanotubes: Their Properties and Applications* (Academic, San Diego, 1996).
[2] P. Moriarty, Rep. Prog. Phys. 64, 297 (2001).
[3] G.Fugallo et al *Thermal conductivity of graphene and graphite: collective excitations and mean free paths* Nano Lett. 14 (11), 6109(2014)
[4] T. Kang et al. *Ultrafast nonlinear phonon response of few-layer hexagonal boron nitride* PRB-L 104 (14), L140302(2021).
[5] C. Melis et al. *Room Temperature Second Sound in Cumulene* PCCP. 23, 15275-15281 (2021)
[6] G. Fugallo et al. *Infrared reflectance, transmittance, and emittance spectra from first principles* PRB 98 (18), 184307 (2018)
[7] G. Cassabois et al. *Superradiance of optical phonons in two-dimensional materials* Phys Rev. Research 4 (3), L032040 (2022)
[8] G. Cassabois et al. *Exciton and phonon radiative linewidths in monolayer boron nitride* PRX 12 (1), 011057 (2022)

Thermal transfert through interfaces and close to free surfaces via atomistic simulations

Konstantinos TERMENTZIDIS
[1]*CETHIL, Centre for Energy and Thermal Sciences of Lyon, CNRS, INSA of Lyon, France*
*corresponding author: konstantinos.termentzidis@insa-lyon.fr

The revolution of nanomaterials elaboration methods the last decades emerge new class of nanostructures and nanostructured materials like phononic-like crystals [1], crystalline/amorphous nanocomposites [2] and superlattices [3,4], nanowire networks [5], assymetric nanostrucures, etc. The drastic reduction of the thermal transport in the majority of these materials and the particular transport effects observed recently both in experimental and theoretical studies are related to the domination of interfaces and surfaces and of their densification to the heat dissipation. These modifications are related to phonon confinement and boundary scattering, as well as to new physical phenomena as ballistic phonon transport, phonon diffraction and interference [6], phonon tunneling [2], coherence effects, thermo-hydo-dynamic flow [7], rectification effects [8] etc. Physical insights of such phenomena will be presented here in several nanometric systems extracted from Molecular Dynamics Simulations and wave propagation simulations.

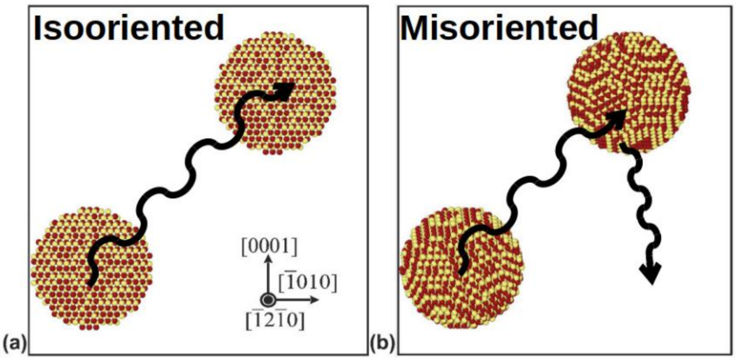


Fig.1. Schematic representation of the phonon percolation within neighboring crystalline GaN nanoinclusions inside an amorphous SiO2 matrix for two cases: isooriented and misoriented growth direction of nanoinclusions. [XX]

[1] M. Verdier et al, Phys. Rev. B **97**, 115435 (2018).
[2] K. Termentzidis et al, Nanoscale **10**, 21732 (2018)
[3] A. France_Lannord et al, J. Phys. Cond. Matt. **26**, 355801 (2014).
[4] P. Desmarchelier et al, J. Appl. Phys. **134**, 185105 (2023).
[5] M. Verdier, D. Lacroix and K. Termentzidis et al, Phys. Rev. B **98**, 155434 (2018)
[6] P. Desmarchelier et al, J. Appl. Phys. **135**, 015103 (2024).
[7] P. Desmarchelier et al, Int. J. Heat and Mass Trans. **194**, 123003 (2022).
[8] P. Desmarchelier, A. Tanguy, and K. Termentzidis, Phys. Rev. B **103**, 014202 (2021).

Real-time observation of III-V nanowire growth by in-situ TEM

Federico Panciera,[1]* Chen Wei,[1] Qiang Yu,[1] Nam Hong,[1] Zhaslan Baraissov,[2] H. Saidov,[3] Gilles Patriarche,[1] Vladimir G. Dubrovskii,[3] Frank Glas,[1] Utkur Mirsaidov,[2] Jean-Christophe Harmand,[1] Laurent Travers[1]

[1]*Université Paris-Saclay, CNRS, Centre de Nanosciences et de Nanotechnologies, 91120, Palaiseau, France.*
[2]*Centre for BioImaging Sciences, Department of Biological Sciences, National University of Singapore, 14 Science Drive 4, 117557, Singapore*
[3]*ITMO University, Kronverkskiy pr. 49, 197101 St. Petersburg, Russia*

*Corresponding author: federico.panciera@c2n.upsaclay.fr

Here, we present experimental observations of the growth of self-catalyzed and Au-catalyzed III-V nanowires using a transmission electron microscope (TEM). Nanowires are grown directly inside the microscope, and their growth is monitored in situ and in real-time with high spatial and temporal resolution. We will present direct observations of the main steps of nanowire growth, from catalyst deposition to crystal nucleation and growth. We will then investigate the control of the crystal phase in III-V nanowires. Bulk semiconductors generally exist in only one crystal phase, but at the nanoscale, multiple crystal phases can coexist. This occurs, for example, when GaAs nanowires are grown using the vapor-liquid-solid (VLS) method. In these nanowires, the stable zincblende (ZB) phase coexists with metastable wurtzite (WZ) structure, resulting in nanowires having a mixed-phase structure. Remarkably, the valence and conduction bands of the two phases are misaligned so that small sections of one phase within the other effectively confine charge carriers. These heterostructures are defined as crystal-phase quantum dots (CPQDs) and have been proposed for several potential applications in photonics and quantum computing [1-3]. Moreover, in contrast to compositional heterojunctions, CPQDs have intrinsically strain-free and abrupt interfaces, hence do not suffer from alloy intermixing, which hampers precise control of the electronic properties in compositional heterostructures. The technological application of CPQDs has been severely limited by the poor understanding of the phase selection mechanism and the difficulty of controlling their formation. Only recently, thanks to in situ TEM, could we shed new light on the phase selection mechanism and demonstrate how to achieve structural control. In fact, in situ TEM provides unparalleled imaging resolution and allows one to capture in real-time the growth dynamics and the effects of changing growth parameters [3,4,5]. The importance of the nanowire-catalyst interface and contact angle between the liquid droplet and nanowire was pointed out theoretically early on. It is, however, only by using in situ TEM that we could demonstrate that the phase selection can be controlled by simply tuning the contact angle [6,7]. These findings are explained within a dedicated model based on surface energetics and provide a clear route for the crystal phase control in III-V nanowires.

[1] Akopian *et al.* Crystal phase quantum dots. Nano Lett. 2010, 10 (4), 1198-1201.

[2] Li *et al.* Location Qubits in a Multiple-Quantum-Dot System. Nano Lett. 2024, 24 (18), 5656–5661.

[3] Loitsch *et al.* Crystal phase quantum dots in the ultrathin core of GaAs–AlGaAs core-shell nanowires. Nano Lett. 2015, 15(11), 7544-7551.

[4] Harmand *et al.* Atomic step flow on a nanofacet. Phys. Rev. Lett. 2018, 121, 166101.

[5] Glass *et al.* Statistics of Nucleation and Growth of Single Monolayers in Nanowires: Towards a Deterministic Regime. *physica status solidi (RRL)*, 2022, *16*(5), 2100647.

[6] Jacobsson, *et al.* Interface dynamics and crystal phase switching in GaAs nanowires. Nature, 2016, 531, 317-322.

[7] Panciera *et al.* Phase selection in self-catalyzed GaAs nanowires. Nano Lett. 2020, 20(3), 1669-1675.

Comment piloter la morphologie de couches métalliques ultra-minces ?
Apport des mesures in situ et en temps réel durant et après la croissance

G. Abadias[1]*, K. Solanki[1], M. Kaminski[2], B. Krause[2], A. Michel[1], A. Vlad[3], A. Resta[3],
Y. Garreau[3], A. Coati[3], D. Babonneau[1]
[1]*Institut Pprime, CNRS-Université de Poitiers-ENSMA, Chasseneuil-Futuroscope, France*
[2]*Karlsruhe Institute of Technology, Karlsruhe, Allemagne*
[3]*Synchrotron SOLEIL, Saclay, France*
*corresponding author: gregory.abadias@univ-poitiers.fr

Les couches métalliques ultrafines (épaisseur ~ 10 nm) sont omniprésentes dans de nombreuses applications optoélectroniques. L'argent (Ag) est de loin le matériau de choix pour un certain nombre de domaines technologiques clés, citons par exemple les vitrages à basse émissivité, les émetteurs thermiques infrarouges sélectifs pour le refroidissement radiatif ou encore les électrodes transparentes conductrices (TCE) pour les systèmes photovoltaïques flexibles. Cependant, la tendance naturelle de l'Ag est de croître sous formes d'îlots 3D (mode Volmer-Weber) sur de nombreux substrats. Des stratégies visant à produire des couches d'Ag continues, ultrafines et ultra-lisses sans compromettre leur conductivité électrique ont récemment été déployées. Parmi elles, l'utilisation d'additifs gazeux, tels que N_2 ou O_2, ou de couches buffers semble être une voie efficace pour améliorer le mouillage de l'Ag et favoriser une morphologie de croissance 2D [1-3]. De plus, du fait de la forte mobilité de l'argent, les morphologies des couches observées post-dépôt diffèrent généralement de celles en cours de croissance. Ainsi, afin de comprendre la dynamique de croissance de ces films, notamment lors des premiers stades (nucléation, coalescence et formation d'une couche continue) la mise en œuvre de diagnostics *in situ* et en temps réel est primordiale.

Nous avons développé au cours des dernières années une approche expérimentale originale, couplant plusieurs caractérisations complémentaires in situ pendant la croissance, notamment à partir de la courbure du substrat, résistivité électrique et réflectivité différentielle de surface (SDRS) accessibles en laboratoire, et étendues à des expériences utilisant le rayonnement synchrotron (diffraction/diffusion des rayons X), voir Figure 1. Nous présenterons dans cet exposé les résultats obtenus lors de la croissance par pulvérisation magnétron de films ultraminces d'Ag, à savoir l'influence de la réactivité du substrat (SiO_x, SiN_x, Ge) et de la présence d'azote (N_2) introduit dans le plasma sur les morphologies de croissance. Nous discuterons également les évolutions lors d'une interruption de croissance à différents stades, avant et après percolation et dans le cas de couches continues.

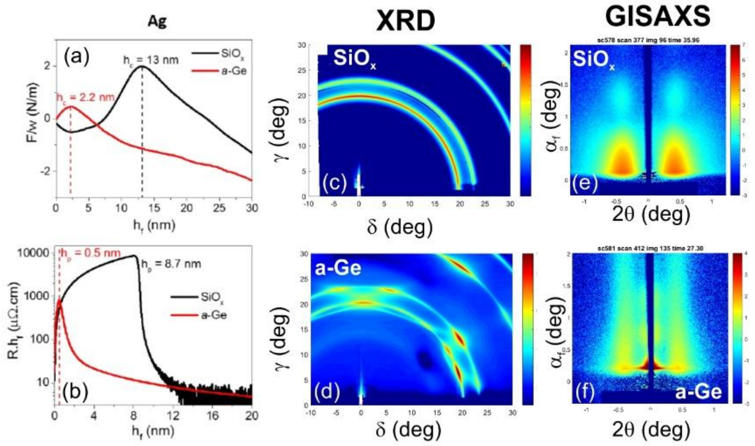


Fig. 1: Mesures en temps réel de la courbure du substrat (a) et résistivité électrique (b) lors de la croissance de Ag/SiO_x et Ag/a-Ge. On observe une diminution des épaisseurs de percolation (0.5 vs. 8.7 nm) et continuité (2.2 vs. 13 nm) dans le cas Ag/a-Ge. Les mesures GISAXS (e et f) confirment ces modifications morphologiques lors des premiers stades, qui se traduisent aussi par une amélioration de la texture des couches d'Ag à plus forte épaisseur (c et d).

Ces travaux s'inscrivent dans le cadre du projet PRCI IRMA financé par l'ANR et du projet DREAM financé par la Région Nouvelle Aquitaine.

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Structure et Propriétés des Interfaces Semiconductrices : Une approche atomistique et multi-échelle

A. Hémeryck[1]
[1]*Laboratoire d'Analyse et d'Architecture des Systèmes, LAAS-CNRS, Université de Toulouse, CNRS, Toulouse, France*
*corresponding author: anne.hemeryck@laas.fr

Les interfaces semiconductrices sont des éléments clés dans de nombreux dispositifs fonctionnels avancés. Leur compréhension requiert une approche intégrant plusieurs échelles de temps et d'espace, ainsi que des outils de simulation variés pour appréhender des mécanismes complexes tels que la diffusion atomique, les réactions chimiques ou encore les transitions de phase.

Dans ce cadre, mon travail s'appuie sur une combinaison de méthodes atomistiques (DFT, dynamique moléculaire, Activation-Relaxation Technique [1]) et mésoscopiques (Monte Carlo cinétique [2]). Ainsi que le recours aux approches d'apprentissage machine [3]. Cette synergie permet de surmonter les limites individuelles de chaque méthode et de traiter des problématiques variées, comme la présence d'impuretés aux interfaces amorphes/cristallines [4], l'interdiffusion conduisant à la formation de siliciures ou d'alliages [5], ou encore le contrôle des interfaces parfaites pour des matériaux topologiques [6].

Ces exemples illustrent la complexité inhérente à l'étude des interfaces, où chaque phénomène est lié à des échelles distinctes, nécessitant une modélisation fine et multi-niveaux. Ces résultats offrent de nouvelles perspectives pour l'ingénierie des interfaces dans les nanomatériaux, avec des applications potentielles dans l'électronique et les nanotechnologies.

[1] **Exploring potential energy surfaces to reach saddle points above convex regions** - Miha Gunde, Antoine Jay, Matic Poberznik, Nicolas Salles, Nicolas Richard, Georges Landa, Normand Mousseau, Layla Martin Samos, Anne Hémeryck, *The Journal of Chemical Physics* **160** (2024) 232501 - doi: https://doi.org/10.1063/5.0210097

[2] **Kinetic Monte Carlo for Process Simulation : First Principles Calibrated Parameters for BO2 Complex** - Pierre-Louis Julliard, Antoine Jay, Miha Gunde, Nicolas Salles, Frédéric Monsieur, T. Cabout, Nicolas Guitard, Layla Martin-Samos, Denis Rideau, Fuccio Cristiano, Anne Hémeryck - *2021 International Conference on Simulation of Semiconductor Processes and Devices (SISPAD)* (2021) pp. 219-223 - doi: 10.1109/SISPAD54002.2021.9592580

[3] **Developing a Neural Network Potential to Investigate Interface Phenomena in Solid Phase Epitaxy** - Ruggero Lot, Layla Martin-Samos, Stefano De Gironcoli, Anne Hémeryck - *2021 IEEE 16th Nanotechnology Materials and Devices Conference (NMDC)* (2021) pp. 1-5 - doi: 10.1109/NMDC50713.2021.9677541

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[6] **Growth modes of BiSb on GaAs (001) versus (111)A surfaces: experimental and theoretical study -** Dima Sadek, Antoine Jay, Jihan El Hila, Rémi Démoulin, Fuccio Cristiano, Sébastien Plissard, Anne Hémeryck - *Applied Surface Science* **622** (2023) 156688 - doi: 10.1016/j.apsusc.2023.156688

Ab Initio Models of Functionalized Gold Nanoparticles and Self-Assembled Monolayers on Gold Surfaces for Various Applications

David Loffreda[1]
[1]*ENSL, CNRS, Laboratoire de Chimie UMR 5182, 46 Allée d'Italie, 69364 Lyon Cedex, France*
*corresponding author: david.loffreda@ens-lyon.fr

Designing functionalized gold nanoparticles and surfaces at the atomic scale remains a tremendous challenge, although such a requirement may be necessary for various applications in biomedicine, biosensors, optics, transistors, catalysis etc. From the experimental standpoint, significant efforts have been made over the years to acquire knowledge on the relationships between the morphology of gold nanoparticles and their chemical environment, or between self-assembled monolayers and the targeted properties. However, it remains necessary to better understand what direct and indirect physical phenomena are at stake, when gold nanoparticles and surfaces are interacting with their nearby chemical environment. Theoretical modeling at a sufficient level of accuracy may be an interesting approach to progress on these questions. In this presentation, several examples showing the impact of the environment on the morphology of gold nanoparticles will be exposed thanks to close collaborations with experimentalists and theoreticians [1-3]. In particular, the influence of the hydration, the PEGylation, the high pressure of hydrogen on gold structures will be evoked on the basis of density functional theory calculations and *ab initio* molecular dynamics simulations.

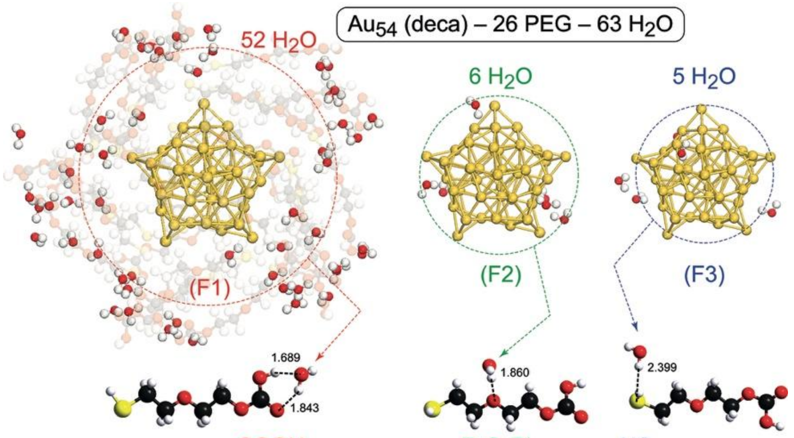

Fig.1. Figure. PEGylated and hydrated Au54 regular decahedron optimized by DFT. The observed stellation leads to a more ordered organization of the organic layer (of the "regular brush" type)

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Non-thermal desorptions of molecular ices: on the trail of mechanisms

D. Torres-Díaz[1,2], R. Basalgète[2], A. Hacquard[2], G. Féraud[2], X. Michaut[2], L. Philippe[2], J.-H. Fillion[2], M. Bertin[2], L. Amiaud[1], A. Lafosse[1*]
[1] *ISMO, CNRS, Université Paris-Saclay, France*
[2] *MONARIS, Sorbonne Université, Paris, France*
*corresponding author: anne.lafosse@universite-paris-saclay.fr

In the coldest regions (10 K – 100 K) of the interstellar medium, where stars and planet are formed, molecular matter mostly exist in the solid phase, forming ices on the surface of dust grains. However, several molecules have been detected in the gas phase in quantities that cannot be explained without considering non-thermal desorption mechanisms [1,2]. Among these mechanisms, photon-induced desorption has been widely studied, especially UV-induced desorption and, more recently, X-ray-induced desorption. Our aims are to evaluate the efficiency of these processes by measuring quantitative desorption yields, to assess the contribution of electron-induced processes to the photodesorption, and to better understand the complex chemistry in icy mantles, as illustrated in figure 1.

Molecular ices were grown at cryogenic temperatures (15-100 K) and under ultra-high vacuum conditions. They were irradiated either in the core-shell or in the valence-shell energy range to induce desorption with the monochromatic output of synchrotron beamlines (DESIRS & SEXTANTS) at SOLEIL using the SPICES setup (MONARIS) or with electrons in the SOMO setup (ISMO). The desorbing neutral species were analysed and quantified during irradiation using mass spectrometry. Temperature-programmed desorption (TPD) was used to calibrate the desorption signal and the ice thickness, and as a post-irradiation analysis of the ice. Desorption efficiencies per incident/absorbed particle were measured as a function of incident energy in the low-dose regime (spectroscopic study), as a function of cumulative dose at a fixed irradiation energy (kinetic study), and as a function of the icy film thickness [3].

An interesting complementarity was obtained between the laboratory's flexible electron irradiation experiments and those carried out at the synchrotron on model molecular ices of methanol CH_3OH [4,5], ammonia NH_3 [3,6] and acetonitrile CH_3CN [3,7].

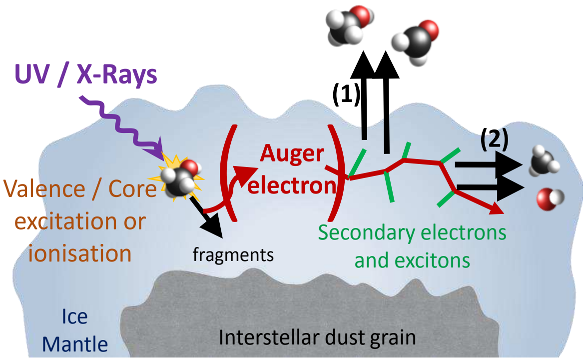

Fig.1. Scheme of processes taking place in the ice after photon absorption.

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Biocompatible and biomimetic droplets to probe tissue mechanics

L.-L. Pontani

Laboratoire Jean Perrin, Sorbonne Université, CNRS, Institut de Biologie Paris-Seine (IBPS),

Emulsions, i.e. packings of oil droplets in water, are a great tool to explore the structure of jammed matter. Indeed, contrary to classical granular systems, emulsions can be made transparent, allowing to image their 3D structure through classical microscopy techniques. It is then possible to study straightforwardly how the packing structure depends on parameters such as the size distribution of the droplets, their interactions, or an applied pressure.

Beyond these approaches, emulsions can also be tuned to exhibit properties that resemble those of biological tissues, with the general goal to understand the physical basis of collective remodeling during development. These biomimetic emulsions are designed to mimic the minimal mechanical and adhesive properties of cells in biological tissues. Such a biomimetic approach allows to study the mechanical properties of tissues in a simplified framework, i.e. a framework in which the inherent biological complexity due to intracellular regulations is bypassed. In particular, we focus on the interplay between adhesion and mechanical forces and how it regulates the emergence of tissue architecture during morphogenesis. To do so, we first studied the elasto-plasticity of these emulsions as a function of interdroplet adhesion and showed that adhesion alone was able to guide the emergence of structuration in biomimetic emulsions.

In parallel to this in vitro approach, droplets can be used to probe cellular forces inside biological environments. Indeed, droplets can be made soft enough to probe forces exerted by cells or tissues: knowing their surface tension, it is then possible to quantify the local exerted stress from their observed deformation. We are currently using droplets to unravel the role of the extracellular matrix in the mechanical coupling of cells and tissues during morphogenesis.

Structure, molecular confinement and photocatalysis applications in geo-inspired clay nanotubes

E. Paineau[1]

[1]*Laboratoire de Physique des Solides, CNRS/Université Paris-Saclay, Orsay, France*

*corresponding author: erwan-nicolas.paineau-lanone@cnrs.fr

Hollow cylinders with a diameter in the nanometer range are carving out prime positions in nanosciences. Thanks to their physico-chemical properties, they could be key elements for next-generation nanofluidics devices, for selective molecular sieving, energy conversion or as catalytic nanoreactors. Some challenges such as diameter and interface control are solved for imogolite nanotubes (INTs). Belonging to clay minerals, imogolite exists in its natural state but is widely dispersed in environment, limiting its applications. The major breakthrough for using INTs was certainly their synthesis by sol-gel methods under mild conditions.

We will first focus here on the recent developments of imogolite nanotube synthesis, particularly in terms of morphological control and surface functionalization [1]. We will show that it is now possible designing innovative geo-inspired INTs with modular interfaces in a predictive way, which has recently led to some progress in the field of imogolite-based functional materials and liquid-crystals [2,3]. We will also prove that this system is ideal to investigate the structure and dynamics of water in interaction with the nanotube walls [4]. Furthermore, the imogolite structure leads to a permanent intrawall polarization arising from the presence of bifunctional surfaces at the inner and outer tube walls. Density functional theory simulations suggest such bifunctionality to encompass also spatially separated band edges [1] (Fig. 1). We will illustrate that INTs are appealing candidates for facilitating chemical conversion reactions and could be considered as potential photoactive nanoreactors [5,6].

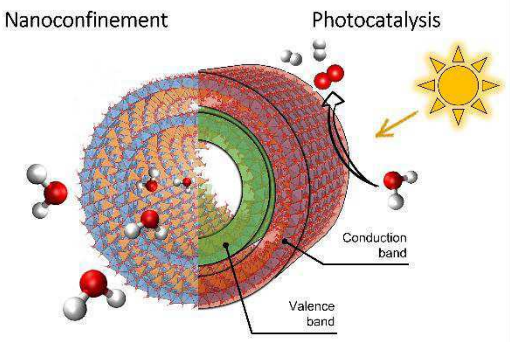

Fig.1. Schematic illustration of the combined confinement and photocatalysis applications in imogolite nanotubes.

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Manipulation of magnetic skyrmions for memory and logic applications

O. Boulle[1]

[1]*Spintec, Grenoble, France*

Magnetic skyrmions are magnetic nanoscale bubbles which are envisioned as bits of informations in our computers. This magnetic quasi-particle can reach sizes down to a few nanometers, and is composed of elementary nanomagnets (spins) that wrap to form a very stable spiral structure, like a tightly-knit knot. Several memory and logic devices have been proposed based on magnetic skyrmions, promising very high information density and low energy consumption. These devices are based on the manipulation of skyrmions in magnetic tracks by an electric current. However, such applications remained distant, as the magnetic moment of skyrmions limits their speed to 100 m/s - too slow for applications - and leads to a deflection of the skyrmions' motion towards the edge of the track, where they can annihilate.

In this presentation, I will show that these limitations can be overcome in synthetic antiferromagnetic materials. These materials consist of two nanometer-thick ferromagnetic layers (such as cobalt), separated by a thin non-magnetic layer, with opposite magnetizations. The skyrmions in synthetic antiferromagnets are composed of two skyrmions whose spins are aligned in an opposite direction, thus cancelling out the magnetic moment (Figure 1, left). Our team has shown that skyrmions in these materials can be moved by electric currents almost ten times faster than ferromagnetic materials, up to 900 m/s, and along the direction of the current (see Figure 1, right). The experimental results are in good agreement with the predictions of theoretical and numerical models. These results were recently published in the journal Science [1]. I will also show that skyrmions can be detected electrically with high electrical signal in magnetic tunnel junctions [2]. The next step will be to perform memory and logic operations based on skyrmion train manipulation in these materials, a step closer to using these new particles to encode and manipulate information at the nanoscale.

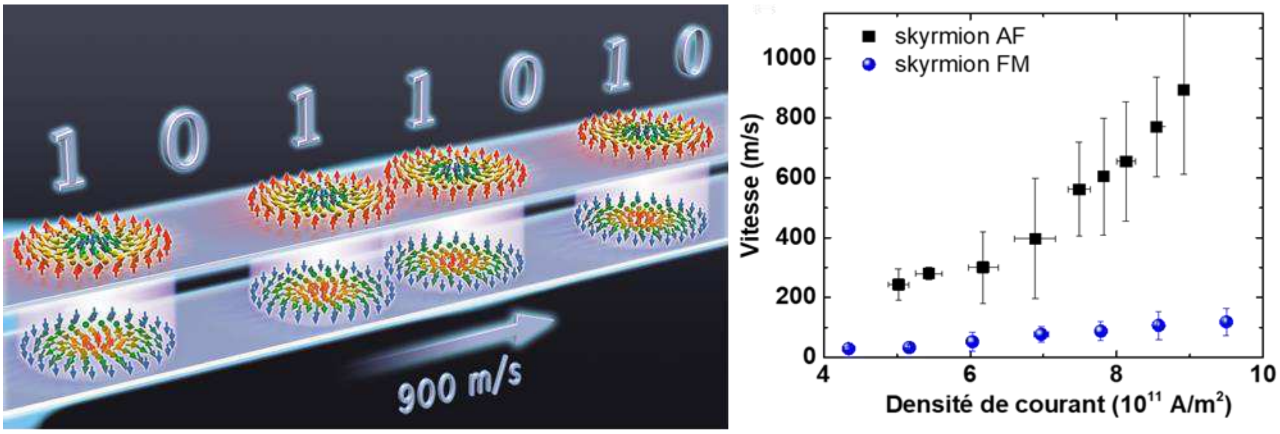

Figure 1 Left Skyrmions in synthetic antiferromagnets are composed of two skyrmions whose spins are aligned in opposite directions. Right Skyrmion velocity as a function of injected current density for skyrmions in SAF (black squares) and in single ferromagnetic

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Ferroelectric and antiferroelectric materials: dielectric properties and applications

C. Borderon
IETR, UMR CNRS 6164, Nantes University, 44322 Nantes, France
corresponding author: caroline.borderon@univ-nantes.fr

Ferroelectric and antiferroelectric materials have spontaneous polarization. Their dielectric properties are therefore nonlinear, which makes them suitable for different applications. Ferroelectric materials are thus used for FeRAMs but also in microwave devices because the polarization defines the permittivity ε as:

$$\varepsilon = \frac{dP}{dE}$$

Since polarization describes a hysteresis loop, the permittivity is not constant and varies with the applied electric field. This property is often exploited to create voltage-tunable capacitances for microwave devices. However, the derivative of the polarization loop does not perfectly match measurements of dielectric permittivity taken with a DC bias electric field. This discrepancy highlights the importance of considering the dependencies of permittivity on both frequency and the amplitude of the applied field, as well as the distinct contributions within the material: switching contribution, lattice or domain wall motions. At low excitation fields, for example, variations in permittivity are primarily due to domain wall motions and can be described by a hyperbolic law [2]. This approach reveals the lattice's contribution to permittivity and the effects of domain wall vibration and pinning/unpinning. Additionally, this analysis provides insight into domain wall density and the depth of the pinning potential. At higher electric fields, permittivity decreases due to coalescence of domains, reducing domain wall density, a process associated with polarization switching. Polarization switching can be further examined using First-Order Reversal Curve (FORC) measurements, which decompose the complete polarization loop *P*(*E*) into elementary hysteresis components (hysterons). This decomposition provides detailed information on fatigue [3-4] and degradation of ferroelectric polarization. Moreover, FORC is particularly useful for distinguishing residual ferroelectric phases in antiferroelectric materials [5].

The present contribution gives an overview on dielectric properties, which allows us a description of the polarization switching dynamics of ferroelectric and antiferroelectric materials. All properties are explained with examples of applications to understand how to improve ferroelectric and antiferroelectric materials.

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Ferroelectric materials in the light of synchrotron X-ray diffraction

T.W. Cornelius[1]
[1] *Aix-Marseille Université, Université de Toulon, CNRS, IM2NP, Marseille, France*
*corresponding author: thomas.cornelius@im2np.fr

Piezoelectric transducers, which convert electrical energy into mechanical energy (and vice-versa) are widely used in several applications for communication, sensing and energy harvesting. Piezoelectric materials are thus integrated in various devices, including resonators, actuators and sensors, more recently in thin film form for their integration into microelectronic devices and for miniaturization purposes (at lowest energy consumption). It is well established that the piezoelectric coupling coefficients are very large in crystalline materials which are also ferroelectric, *i.e.* which exhibit a remanent electrical polarization, switchable by applying an external electric field. In particular, the presence of ferroelectric domains contributes to this large piezoelectric effect. These domains are regions in which the orientation of the polarization vector and the spontaneous strain tensor are uniform, separated by domain walls. The domain structure is strongly affected by the strain in the thin films and by the electrical boundary conditions, which depend on both bottom and top electrodes. The polarization switching mechanism is typically in the nanosecond range, but the domain dynamics under applied electric field, including domain nucleation and lateral growth, is affected by the domain structure and the presence of nearby domain walls.

Here, we present *in situ* and time-resolved synchrotron X-ray diffraction studies on ferroelectric thin films during the application of an electric field [1-3]. It grants strain resolutions of the piezoelectrically-induced strain of better than 10^{-4} and temporal resolutions of the domain switching dynamics of few tens of nanoseconds. In addition, nanofocused scanning X-ray diffraction mapping allows for probing the strain field in the vicinity of domain walls [4].

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Opto-electric control of van der Waals ferroelectric heterostructures : opportunities for beyond-Moore applications

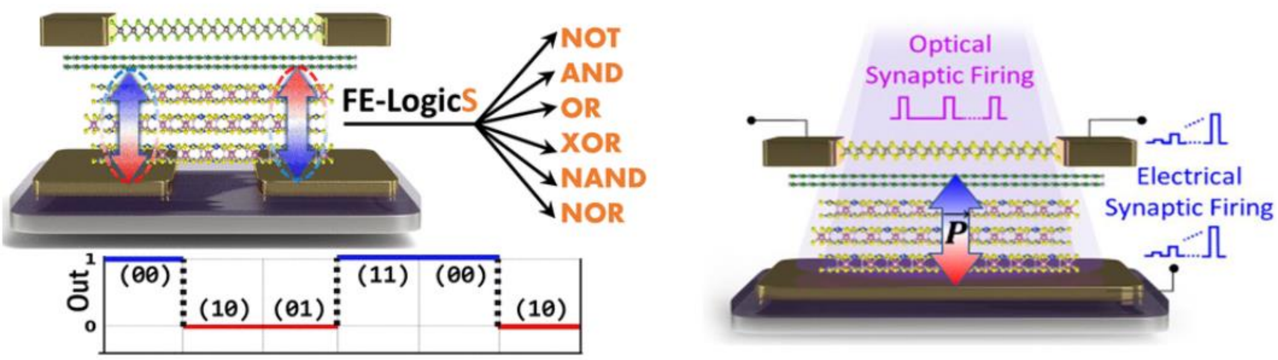
Jean-François Dayen
[1]*Université de Strasbourg/CNRS/Institut de Physique et de Chimie des Matériaux de Strasbourg,*
*corresponding author: dayen@unistra.fr

Two dimensional ferroelectric materials are attracting fast growing interest for the implementation of complex architectures and enhanced functionalities, going beyond standard thin film technology.**[1]** Today, I will present recent developments on the coupling of a 2D van der Waals (vdW) electron gas with various ferroelectric gate controls. We will discuss how these systems allow for rethinking circuit topology and memory-logic interaction, opening up new research directions in the area of frugal computational enhancement and neuromorphic computing for AI.

I will first detail how by making use of the switchable polarization state of two split ferroelectric gates, the electrical potential landscape within 2D semiconductor channel can be engineered with non-volatile state and real-time reconfigurability. **[2]** While using the non-volatile ferroelectric states as logic parameters, the ferroelectric logic circuits can function as six alternative logic gates, while CMOS circuit are limited to a single function. Such reconfigurable FeFET circuits demonstrate high compactness, with an up to 80% reduction in transistor count compared to standard CMOS design. Moreover, the device can operate as a photodiode and generate photovoltaic energy.

Finally, I will present how light-structure interactions in vdW systems allow for implementing the non-volatile electrical and optical control of the ferroelectric polarization in ferroelectric/semiconductor heterostructures. **[3]** The wavelength-dependent study unveils ferroelectric polarization control and decouples the mechanisms driven by photogenerated carriers for each material and at the interfaces. Following, long-term potentiation/depression, and spike rate-dependent plasticity are shown using both electrical and optical controls, enabling optically stimulated and optically assisted synaptic devices.

These studies aim to provide valuable insights into the opto-electronic processing of ferroelectric states, their encoding into non-volatile multiple states, and their manipulation for neuromorphic and in-memory computing technologies.



Schematics of van der Waals ferroelectric devices. Left: Reconfigurable ferroelectric logics. Right: Photoferroelectric Artificial Synapse.

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Optical spectroscopy of excitons in 2D semiconductors

Fabian Cadiz
Laboratoire PMC, Ecole polytechnique

Currently, one of the main research topics in condensed matter physics deals with the electronic properties of atomically thin semiconductors based on transition metal dichalcogenides (TMD), such as MoS_2 and WSe_2.

Due to quantum confinement and weak dielectric screening in their monolayer form, the optical response is completely dominated by strongly bound excitons even at room temperature. Their strong coupling with light permits to study exciton and many body physics through simple photoluminescence experiments. In addition, their unique bandstructure provides the possibility to optically control the electron's spin and wavevector by using circularly polarized light.

In this talk, I will show how optical spectroscopy can provide very useful insights on the bandstructure of these 2D semiconductors.

Interlayer coupling and twist angle in 2D van der Waals systems: An STM approach

P. Mallet
Institut Néel, CNRS & Université Grenoble Alpes, 38000 Grenoble, France

pierre.mallet@neel.cnrs.fr

Two-dimensional van der Waals (vdW) heterostructures have become very attractive in the last decade, thanks to the high tunability of their (opto)-electronic properties. In particular, the interlayer vdW interaction offers unique opportunities of transferring a given property from one layer to the other, through proximity effects [1]. For example, when proximitized with a properly chosen 2D system, it is possible to induce in graphene new properties, such as magnetism or enhanced spin orbit coupling, all lacking in the pristine material [1,2]. Combining magnetic properties and large SOC in graphene is a very active field, related to potential applications in (opto)-spintronics [2].

Recent theoretical works have focused on the interlayer proximity effects between graphene (Gr) and one layer (1L) of a semi-conducting transition metal dichalcogenide. From these calculations, the authors conclude that the interlayer proximity effect, which rely on the hybridization between the electronic states of each layer, is driven by the interlayer twist angle [3-5]. In this talk, I shall review our STM/STS results (complemented by DFT calculations) devoted to that topic, in the case of the monolayer $PtSe_2$/Graphene vdW heterostructure [6], and more recently for the 1L-WSe_2/Graphene system. Our work results from a collaboration with the group of M. Jamet (IRIG/SPINTEC, CEA-Grenoble).

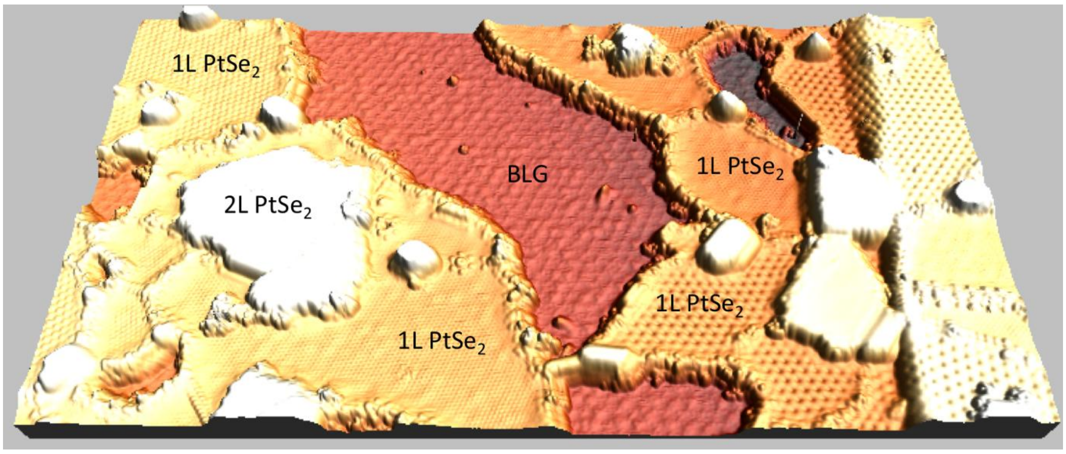

Fig.1. Moiré patterns (related to the interlayer twist-angle) in monolayer $PtSe_2$ islands grown by MBE on bilayer graphene, substrate SiC - Si face. Image size: 110 x 60 nm^2, Sample bias -1.8V

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[2] J. F. Sierra et al., Nat. Nanotechnol. **16**, 856 (2021)
[3] T. Naimer et al., Phys. Rev. B **104**, 195156 (2021)
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Time resolved pump/probe photoelectron spectroscopy: the electronic structure point of view of magnetic phase transitions.

Fausto Sirotti[1]
[1]*Laboratoire de Physique de la Matière Condensée, CNRS-Ecole Polytechnique, IP Paris, Palaiseau, France*
*corresponding author: Fausto.Sirotti@polytechnique.edu

Short laser pump pulses are currently used to induce rapid modifications of magnetic properties. Pump/probe and time resolved photoelectron spectroscopy experiments performed using synchrotron radiation, HHG and free electron laser sources can follow also phase transitions induced by relatively high laser pump fluences, contributing to a better understanding of the observed phenomena. In the most common case, the ferromagnetic order is destroyed and the system becomes paramagnetic. Time scale of the process is strongly related to sample electronic structure [1] and laser fluence. [2] Sometimes, with a temperature increase the system become ferromagnetic. It is the case of FeRh, a metallic material that undergoes a metamagnetic first-order phase transition from antiferromagnetic (AFM) to ferromagnetic (FM) order at 360 K, with coupled structural, magnetic, and electronic order parameters. [3] Experimental (see Fig. 1) and theoretical evidences demonstrate how the modifications induced in the electronic structure drive the magnetic and structural phase transition. [4]

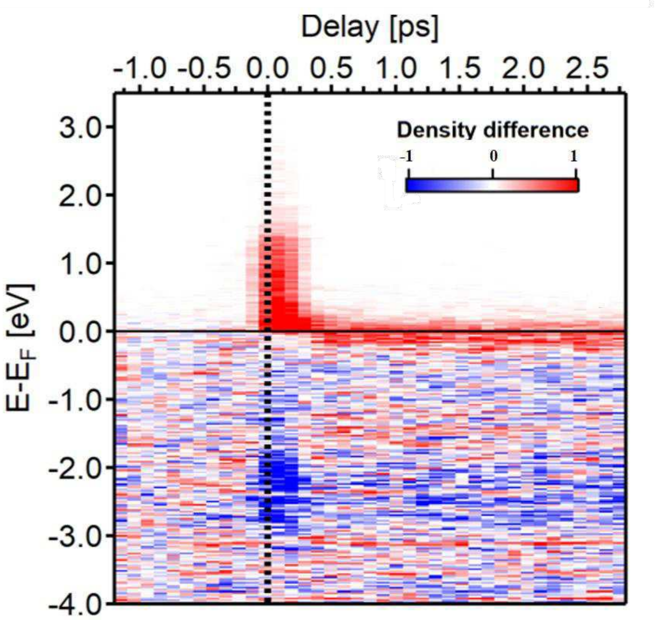

Fig.1. Energy and delay-dependent difference matrix of the photoelectron spectroscopy spectra obtained with a laser pulse excitation at time t=0. The hot electrons appear as an electronic density

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[3] Pressacco, F. et al. Laser induced phase transition in epitaxial FeRh layers studied by pump-probe valence band photoemission. Struct. Dyn. 5, 034501 (2018)

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La spectroscopie de photoémission résolue en angle comme outil unique pour l'étude des propriétés électroniques des solides à l'équilibre et hors-équilibre

G. Kremer[1]

[1]*Institut Jean Lamour, UMR 7198, CNRS-Université de Lorraine, Campus ARTEM, 2 allée André Guinier, BP 50840, 54011 Nancy, France*

*corresponding author: geoffroy.kremer@univ-lorraine.fr

La spectroscopie de photoémission résolue en angle (ARPES) est la technique reine pour accéder aux relations de dispersions dans les solides. Elle est utilisée en laboratoire ou sur de grands instruments pour réaliser des mesures avec une haute résolution énergétique, angulaire, de spin, spatiale ou encore temporelle, que cela soit pour étudier les propriétés électroniques des solides à l'équilibre ou hors-équilibre.

Dans cet exposé, je rappellerai les principes fondamentaux de cette technique et je donnerai un aperçu de ses possibilités et des informations auxquelles elle permet d'accéder. J'illustrerai mon propos avec des mesures de photoémission haute résolution sur des systèmes variés, notamment quasi-bidimensionnels ($IrTe_2$ [1], phosphore noir [2] etc.), et me focaliserai en particulier sur le α-GeTe(111) qui est un semi-conducteur ferroélectrique 3D qui présente le plus gros couplage Rashba parmi les matériaux connus à ce jour. Sa structure électronique dans les états occupés a été largement étudiée par ARPES, notamment résolue en spin (SARPES) [3]. En utilisant la photoémission résolue en temps (tr-ARPES), je montrerai (i) comment accéder à la dispersion de ses états inoccupés dans toute la zone de Brillouin, et (ii) comment il est possible d'induire des effets hors-équilibre conduisant à une augmentation transiente du couplage Rashba à l'échelle de quelques centaines de femtosecondes, que l'on peut suivre de manière dynamique en mesurant la structure de bandes [4]. Par comparaison avec des calculs utilisant la théorie de la fonctionnelle de la densité (DFT), je montrerai que ce changement de structure électronique peut s'interpréter par un déplacement du plan de Ge vers le plan de Te en surface, ce qui signifie une augmentation de la distorsion ferroélectrique photoinduite.

Finalement, si le temps le permet, je montrerai une autre voie pour accéder aux propriétés hors-équilibre des solides. Celle-ci est l'application d'une contrainte mécanique uniaxiale dont on peut suivre les effets sur la structure électronique en utilisant la photoémission. Des résultats particulièrement prometteurs ont montré qu'il est possible d'induire des transitions de phase topologique [5] ou encore de stabiliser certaines phases énergétiquement dégénérées avec d'autres phases à l'équilibre [6] en appliquant une contrainte uniaxiale de l'ordre du %. Je discuterai les limites actuelles, ainsi que les défis qu'il existe concernant l'application de ce type de contrainte avec des mesures d'ARPES haute résolution.

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[2] G. Kremer, M. Rumo, C. Yue, et al., Phys. Rev. B 104, 035125 (2021)
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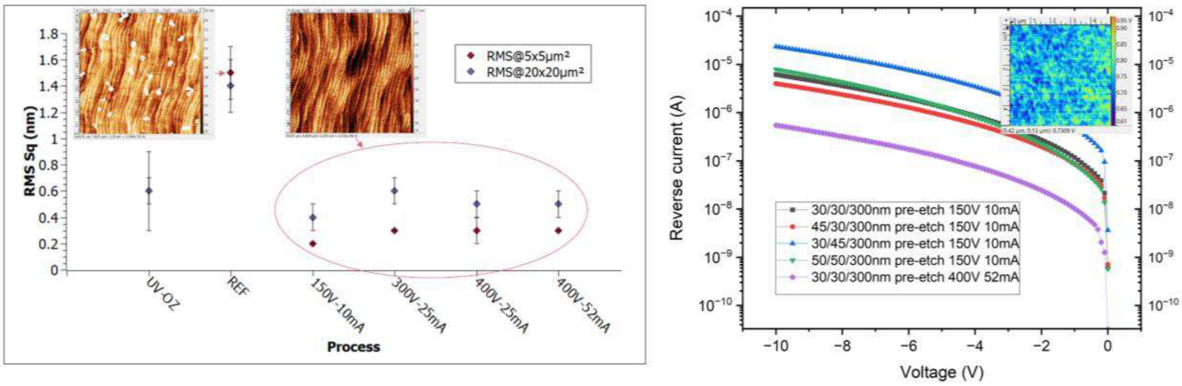
Résumés des posters

How AFM and KPFM analysis of Ar etched n-GaN surfaces relates to leakage current measurements in Schottky barrier diodes

A. Al Abdallah[1,3*], M. Zegaoui[2], L.Thomas[1], E.Okada[1] and M.Zaknoune[1]
[1] *Institut d'Electronique de Microélectronique et de Nanotechnologie, C.N.R.S, Lille, France*
[2] *Research Institute on software and hardware devices for information and Advanced communication, Lille, France*
[3] *Laboratoire d'Etudes du Rayonnement et de la Matière en Astrophysique et Atmosphères, Observatoire de Paris PSL, Paris, France*
*Amir Al Abdallah: amir.alabdallah.etu@univ-lille.fr

Understanding surface states and fermi-level pinning in MOCVD-grown n-GaN is crucial for device applications such as Schottky barrier diodes. Several KPFM studies emphasized the importance of carrier behavior and dislocations [1] on surface potential [2] but no further device fabrication and I-V measurements on the analyzed surfaces have been done to relate to the results. In this study, AFM and KPFM measurements have been done on n-GaN surfaces that were exposed to different etching treatments. Analysis showed etching reduces considerably the RMS value from 1.5nm for the BOE treated surface, taken as reference, to roughly 0.3nm. Measured work functions showed disparities with regard to different etching Bias: the 400V 52mA etched surface was measured to be 0.19V higher than the 150V 10mA surface. Mo-anode Schottky barrier diodes were then fabricated accordingly to the etching configurations of the analyzed surfaces and annealed at 700°C. Leakage currents were measured at -10V and it has been observed that the 400V 52mA pre-etched surface showed a leakage current of 500nA, one order of magnitude less than the moderately pre-etched 150V 10mA diode (4000nA). The potential barriers of the diodes were also extracted from the forward I-V curves and values stand respectively at 0.61eV and 0.57eV.



a) b)

Fig.1. a) Plotted RMS values with regard to different surface treatments. The plotted values are the mean of 3 areas, error bar is standard deviation. Insets in the panel represent 5x5µm² AFM topographies. b) Reverse current of the diodes with regard to different Mo/Pt stacks at the anode junction and two pre-etching extremes; inset is a KPFM map of a 5x5µm² n-GaN surface etched with 400V 52mA Ar ions

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Optimization of Crystalline Structures at CIGS/Metal Oxide Interfaces and Analysis of Their Properties for Improved Solar Cell Performance

Adam Hassan DENAWI, Nicolas Barreau, Isabelle Braems

Nantes Université, CNRS, Institut des Matériaux de Nantes Jean Rouxel, IMN, F-44000 Nantes, France

*Corresponding author: Hassan.DENAWI@cnrs-imn.fr

Solar cells work on the principle of converting light energy into electrical energy and are expected to be a clean and cost effective energy sources. After the first photovoltaic cell was developed at Bell Laboratories in 1954 [1], the research later focused on rather thick silicon wafers (first generation), while Cu(In,Ga)Se_2 (CIGS) thin-film solar cells (second generation) [2,3], have now demonstrated remarkable efficiency and stability over the past two decades. However, the integration within the cell can still be optimized, in particular the electronic and thermodynamical properties of the interface with the back contact are poorly documented in the literature. This is mostly due to the experimental difficulties to characterize such hetero-interfaces at the atomic scale.

My research focuses on optimizing crystalline structures at the hetero-interfaces between recently developed back contacts made of metal oxides and CIGS thin-film solar cells to further enhance their stability and photovoltaic performance. Using *ab initio* simulations based on Density Functional Theory (DFT), we simulate the atomic structures at these interfaces to identify stable configurations and optimize atomic interactions. Furthermore, we investigate the electronic and thermodynamic properties of these interfaces to improve the overall efficiency of CIGS-based solar cells.

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[2] N. Barreau et al., High Efficiency Solar Cell Based on Full PVD Processed Cu(In,Ga)Se_2/$CdIn_2S_4$ Heterojunction, Sol. RRL 1, 1700140 (2017).
[3] J. Wands, A. Bothwell, P. Tsoulka, T. Lepetit, N. Barreau, and A. Rockett, Stability of $Cu(In_xGa_{1-x})Se_2$ Solar Cells Utilizing RbF Postdeposition Treatment under a Sulfur Atmosphere, Adv. Energy Sustain. Res. 4, 2300052 (2023).

1D chains of dye molecules on ultrathin insulators

R. Bretel[1], S. Le Moal[1], H. Oughaddou[1], and E. Le Moal[1]
[1] *Université Paris-Saclay, CNRS, Institut des Sciences Moléculaires d'Orsay, Orsay, France*
*corresponding author: eric.le-moal@universite-paris-saclay.fr

Linear chains of aromatic molecules on thin insulating films are expected to become essential for the study by scanning tunneling microscopy (STM) of the effects of quantum confinement on the electronic and excitonic properties of molecular systems [1,2]. However, until now, such linear chains on thin insulators have only been obtained by assembling the molecules one by one using the tip of an STM, which severely limits the scope of possible investigations and hinders potential applications in device technology. Here, we demonstrate the spontaneous growth of these linear chains by molecular self-assembly on thin insulating films (1 to 3 atomic layers thick) [3]. This growth is particularly challenging due to the weak interactions between the adsorbed molecules and the insulating surface. In this work, we overcome this difficulty by using a prochiral molecule (quinacridone) and an ionic insulator (potassium chloride, KCl). Quinacridone has been shown to self-assemble into homochiral chains on metals, via the formation of hydrogen bonds between neighboring molecules [4]. Furthermore, quinacridone has been shown to be a unique model system for the study of tunneling-induced optical transitions at the submolecular scale [5]. Here, we take advantage of electrostatic interactions between the (partially charged) functional groups of quinacridone and the ions of the underlying KCl layer to stabilize the molecular chains [3]. Using low-temperature STM under ultrahigh vacuum, we determine the molecular arrangement of these chains and their epitaxial relationship with the substrate.

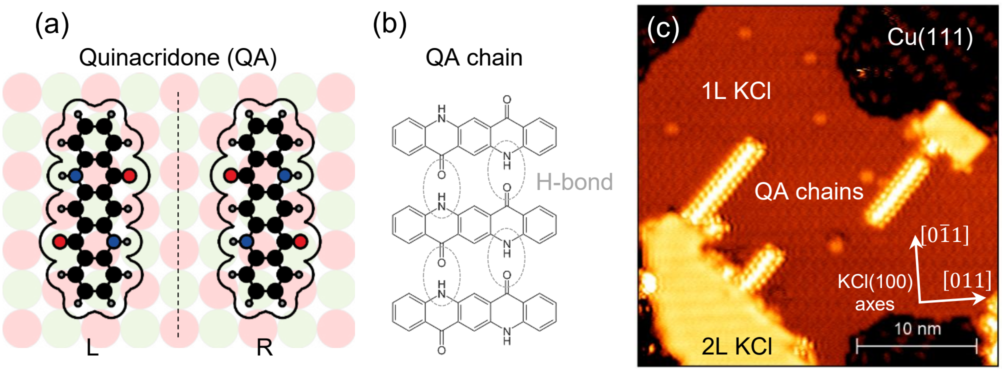

Figure 1: (a) Hard sphere model and van der Waals radii of quinacridone deposited on a KCl(100) surface. The molecule is a prochiral molecule, i.e., depending on which face the molecule adsorbs on a surface, it is one or the other of the two enantiomers (L or R) shown in the figure. (b) Schematic representation of a homochiral (i.e., enantiopure) chain of hydrogen-bonded quinacridone molecules. (c) STM topographic images (4.0 V, 4 pA) of quinacridone molecules deposited on an ultrathin film of KCl on Cu(111). [3].

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[4] N. Humberg et al, J. Phys. Chem. C **124**, 24861 (2020)
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Atomic structure of metallic nanoparticles from EXAFS: transition from monolayer-thick 2D to 3D strained Ag nano-clusters on α-Al_2O_3(0001)

R. Lazzari[1,*], J. Goniakowski[1], G. Cabailh[1], R. Cavalotti[1], J. Jupille[1], N. Trcera[2], P. Lagarde[2]
[1]*Insitut des NanoSciences de Paris, CNRS/Sorbonne Université, 4 Place Jussieu,75005 Paris, France*
[2]*Synchrotron SOLEIL, L'Orme des Merisisers, Départementale 128, 91190 Saint-Aubin, France*
*corresponding author: remi.lazzari@insp.jussieu.fr

Surface and epitaxial stresses play a paramount role in the atomic structure of supported nanoobjects and thereof in their use, such as in the catalytic properties of metal particles. They are suspected to drive transitions of shape [1], of atomic structure and of epitaxy when size is reduced. Nevertheless, x-ray diffraction intrinsically struggles to faithfully characterize clusters in the nanosized regime.

In this context, this poster will report on the interest of coupling x-ray absorption spectroscopy, nanoplasmonics and atomistic calculations in the crystallographic analysis of supported Ag metallic nanoparticles [1-3]. Clusters were grown *in situ* by evaporation on a α-Al_2O_3(0001) surface under ultra-high vacuum and analysed by EXAFS at the Ag L_3 edge to determine the Ag local environment [average Ag-Ag (d_{Ag-Ag}) and Ag-O (d_{Ag-O}) interatomic distances and Ag coordination number (CN)] as a function of the particle size. The experimental key was the capability of a structural study from clusters involving only a few atoms to large nanoparticle obeying the macroscopic equilibrium shape. For large objects, d_{Ag-Ag} is dominated by surface stress and follows the Laplace rule. At sizes below 5 nm, 3D particles in registry on the substrate O sire are partially strained while above interfacial dislocations allow releasing stress. For cluster of a few tens of atoms or less, a transition of registry site from O-top to Al-top is associated to the formation of buckled 2D clusters (Fig. 1), which fingerprint is the concomitant evolution of d_{Ag-Ag} and CN. This finding is unexpected in the light of the poor adhesion at such interface and questions the usual size-independent picture of metal/oxide epitaxy.

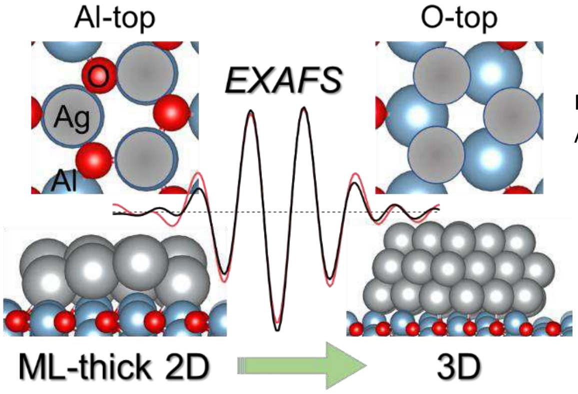

Fig. 1: Transition of registry and dimensionality in epitaxial Ag/α-Al_2O_3(0001) clusters

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Atomic triangulation of the Al_2O_3 layer on a $Ni_3Al(111)$ crystal.

P. Pan[1], A. Ouvrard[1] and P. Roncin[1]
[1] *Institut des Sciences Moléculaires d'Orsay (ISMO), CNRS-Université Paris-Saclay, Orsay, France*

Al_2O_3 /$Ni_3Al(111)$ shows a reconstruction where a missing atom at each corner of the cell leaves possible distant interaction of adsorbates with the metal underlayer providing an powerful nanometric template for the ordered growth of nanoparticles [1]. A sample was prepared accordingly and transferred via a UHV tunnel to a setup for grazing incidence fast atom diffraction (GIFAD) [2] located next room.

The ability of GIFAD to resolve large crystal lattices depends directly on the angular resolution σ_θ of the fast atom beam. With a resolution close to the milli-degree, we could resolve the β_2(2x4) reconstruction of GaAs [3] whose lattice is 16 Å but each improvement of a factor of two reduces the beam intensity by sixteen.

Diffraction is observed only along two directions at 0° and 30° (modulo 60°) but does not allow to resolve the positions of the hundreds of atoms in the lattice cell (see insert). We have complemented these results by an atomic triangulation approach [4] where the width σ_ϕ of the scattering profile of 1 keV helium atoms is recorded during a rotation of the surface around its perpendicular axis (ϕ-scan). σ_ϕ is directly related to the variance σ_m^2 of the intensity of the m diffraction orders [5] but remains well-defined even when no diffraction is observed. Fig.1 shows seven peaks, each revealing a direction where the atoms form alignments generating significant contrast. Using a semi-classical model [6], each peak of this very robust measurement can be related to the width and depth of the channeling valleys of these alignments. More quantitatively, a simple classical diffusion model based on an electron density map as produced by a DFT calculation could be uniquely connected to a triangulation curve. Comparison with experiment could then discriminate different structural models such as the one of ref; [7] for which the DFT generated poschar file is represented in the inset (courtesy of M. Schmid).

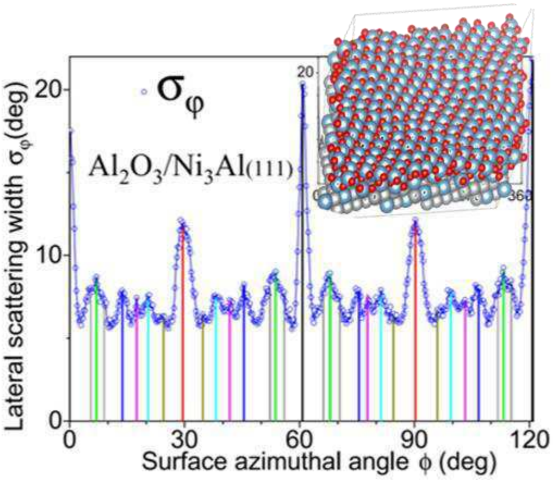

Fig.1 azimuthal scattering width $\sigma_\varphi=\sigma_\phi/\theta$ as a fct of the azimuthal orientation ϕ of the surface.

[1] N. Alyabyeva *et al,* Transition from disordered to long-range ordered nanoparticles Appl Surf Sci p423 (2018)
[2] P. Pan *et al,* A setup for grazing incidence fast atom diffraction, Rev Sci Instrum **93** 093305 (2022},
[3] M.Debiossac *et al* "..fast atom diffraction..on GaAs β_2(2x4)… » Phys. Rev. B **90** 155308 (2014)
[4] N. Kalashnyk and P. Roncin " Atom beam triangulation of organic layers… ." ArXiv 1509.05549 (2015)
[5] $\sigma_\phi = \phi_B * \sigma_m$ where ϕ_B is the Bragg angle associated with the periodicity $a_\perp$; ϕ_B =arctan $k_{//}/G_\perp$; with $k_{//}$ the projectile wavevector // to the surface and $G_\perp = 2\pi/a_\perp$; the reciprocal lattice vector.
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Charge transfer between plasmonic PdAg nanoparticles and C_{60} molecules

Xingtong LI[1], Natalia ALYABYEVA[1], Céline DABLEMONT[1], Aude BAILLY[2], Rémi LAZZARI[3]
and Aimeric OUVRARD[1]
[1]*Institut des Sciences Moléculaires d'Orsay, Université Paris-Saclay, CNRS, 91405, Orsay, France*
[2]*Institut Néel, CNRS, Université Grenoble Alpes et Grenoble INP, 38042, Grenoble, France*
[3]*Institut des NanoSciences de Paris (INSP), CNRS / Sorbonne Université, 75252 Paris, France*
*corresponding author: aimeric.ouvrard@universite-paris-saclay.fr

Understanding the interaction of molecules with a surface or nanoparticles is crucial for effectively control charge transfers in nanoscience. It requires ordered systems where NP and molecules properties can be well controlled [1-3]. We have investigated a hybrid assembly of 2D ordered plasmonic nanoparticles [4] in strong interaction with molecules. It is used as a model system to understand inorganic-organic coupling and particularly the role of the surface plasmon resonance of the nanoparticles on the photophysical properties of the molecule and the charge/energy transfer efficiency and dynamics. Pd/Ag core/shell plasmonic nanoparticles are made by physical vapor deposition in vacuum. NP are then functionalized by C_{60} and their photophysical, plasmonic and vibrational properties are monitored during the growth of C_{60} in real-time by linear and nonlinear optical spectroscopy techniques: Surface Differential Reflectance Spectroscopy (SDRS) and Sum Frequency Generation (SFG). Their structural properties and organization are probed by STM (Scanning Tunneling Microscopy) after the growth.

By tracking SDRS and SFG spectra as a function of time, we observed that during the first 10 minutes of C_{60} deposition, only the changes of surface plasmon resonance are observable. As the deposition time increased, C_{60} vibronic bands appear in the SDRS spectrum. Concurrently, the SFG intensity also starts after 10 minutes and shows a quadratic growth over time, as expected for a second-order optical process. These observations indicates a strong interaction between the nanoparticles and C_{60} molecules. By confronting experimental data to 3D electric field distribution simulated by finite element method (COMSOL), we can propose a growth mechanism and the impact on the coupling of C_{60} with nanoparticles on their optical properties depending on the localisation of the C_{60} on the NP. It opens the way to control charge and energy transfer processes more effectively by driving the position of the molecule in the vicinity of the nanoparticle. Such control is crucial for molecular electronics, photocatalysis, solar cells, and sensors.

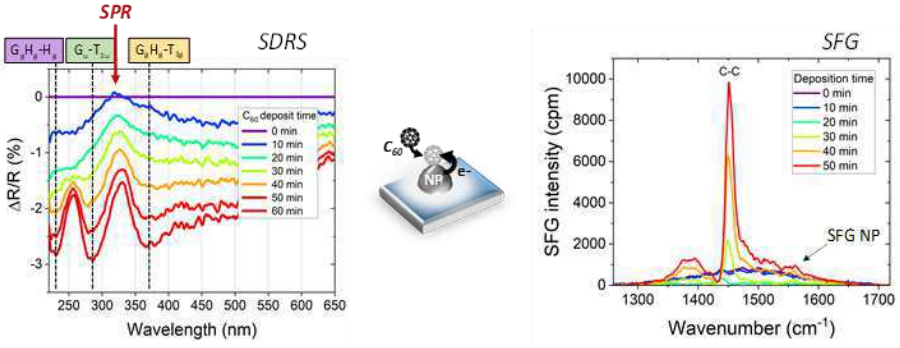

Fig.1. (left) SDRS spectra and (right) SFG spectrum as a function of C_{60} deposition time. (middle) Schematic diagram of C_{60} on NP and the consequent charge transfer.

[1] N. Alyabyeva, A. Ouvrard, A.-M. Zakaria, F. Charra, B. Bourguignon et al., Appl. Surf. Sci, **444**, 423-429 (2018).

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Croissance du Phosphorène sur Vicinales d'Au(111)

W. Ghariani, C. Chacon, A. Karn, J. Lagoute et Y. Girard
Laboratoire Matériaux et Phénomènes Quantiques, Université Paris Cité, Paris, France
W. Ghariani : wissem.ghariani@etu.u-paris.fr

L'étude des matériaux 2D a connu une croissance rapide ces vingt dernières années. Parmi eux, le graphène s'est imposé pour ses propriétés uniques (rigidité, conductivité) et ses applications prometteuses (nano-électronique, stockage de l'énergie). Cependant, d'autres matériaux 2D, mono (silicène, borophène) ou hétéroatomiques (TMD), aux propriétés spécifiques, gagnent également en popularité. Le phosphorène, un plan unique d'atomes de phosphore, émerge ainsi comme une alternative intéressante pour des applications en optoélectronique et en énergie. Récemment, en plus des nombreux allotropes prévus théoriquement **[1]** de nouvelles phases de ce matériau ont été mises en évidence **[2]**, notamment le phosphore poreux **[3].** Au-delà de l'exfoliation du phosphore noir, il s'agit aujourd'hui de synthétiser ces allotropes. Dans ce cadre, nous visons à explorer comment la croissance du phosphore sur des surfaces patternées à l'échelle nano conduit à l'élaboration de nouvelles phases allotropiques de phosphorène précédemment obtenues sur des surfaces métalliques atomiquement planes **[4]**.

Dans cette étude, nous avons évaporé du phosphore sur différentes surfaces d'or, incluant le substrat conventionnel Au(111) ainsi que des substrats vicinaux Au(233) et Au(755). Ces surfaces vicinales, avec leurs réseaux de marches et terrasses périodiques, influencent directement la formation du phosphorène. Nous observons que le phosphore se structure en îlots et en motifs d'écailles de poisson, formant des facettes qui ne se manifestent pas sur Au(111).

Les vicinales d'Au(111), avec leurs terrasses et marches régulières, se révèlent particulièrement adaptées à la formation de formes variées du phosphore bleu (blueP). Ce facettage inattendu est directement relié aux types de bords de marche et signe une profonde restructuration du substrat, ouvrant ainsi un champ d'étude prometteur pour élaborer des formes particulières de phosphorène : ilots, lignes et rubans.

Il s'agit maintenant de déterminer les conditions expérimentales (flux, température, vicinalités) qui favorisent telle ou telle forme de croissance, caractériser leurs propriétés électroniques et leurs arrangements atomiques. Suivant leurs diverses formes, des allotropes particuliers de phosphorène pourraient être privilégiés.

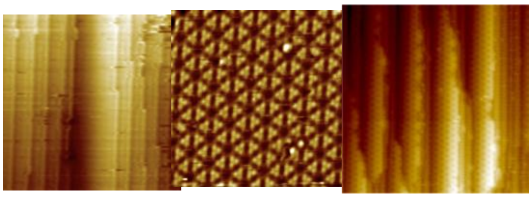

Fig. 1. Images STM de : a) Terrasses de la surface vicinale Au(755), (20x20 nm) ; b) Phosphore bleu (blueP) montrant la structure typique en forme de fleur (10x10 nm) ; c) Phosphore déposé sur un Au(233), révélant la formation de facettes distinctes attribuées au blueP.

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Electric-field-assisted phase switching in GaAs nanowires

Qiang Yu[1], Khalil Hassebi[1], Hakim Saidov[2], Ivan Erofeev[2] Charles Renard[1], Laetitia Vincent[1], Frank Glas[1], Utkur Mirsaidov[2], Federico Panciera[1]

[1] *Université Paris-Saclay, CNRS, Centre de Nanosciences et de Nanotechnologies, 91120, Palaiseau, France.*

[2] *Centre for BioImaging Sciences, Department of Biological Sciences and Physics, National University of Singapore, 14 Science Drive 4, 117557, Singapore*

*Corresponding author email: qiang.yu@universite-paris-saclay.fr

Abstract: The vapor-liquid-solid (VLS) method for nanowires growth was introduced by Wagner and Ellis in the 1960s [1]. Since then, intensive researches focus on engineering the crystal phase of nanowires due to their promising applications in nanotechnology. In nanowires, multiple crystal phases can coexist (polytypism). On the one hand, this phenomenon can be considered as a crystal defect; on the other hand, it enables the formation of crystal phase quantum dots (CPQDs), i.e. insertion of segments of one phase within a nanowire of a different phase. Due to band alignment of two crystal phases and confinement of nanowire size, CPQDs feature single-photon emission and sub-nanosecond exciton lifetime. However, despite over 15-year of research, technological applications of CPQDs remain severely limited by the poor understanding of the phase switching mechanisms and the difficulty of controlling their formation [2]. In this study, beyond commonly used methods of flux and temperature modulation, we solve this issue by introducing an external electric field (E-field) to instantaneously switch the crystal phase and create GaAs CPQDs with monolayer precision. This process is monitored in real-time using in-situ transmission electron microscopy (TEM). Thanks to custom-made substrates, GaAs nanowires are grown epitaxially on Si (111) by chemical vapor deposition. The substrate is shaped as a micro capacitor which allows us to apply an E-filed up to several V/nm in the direction parallel to the nanowire growth, and this strong E-field allows to achieve phase switching faster than monolayer formation. We will present high resolution videos showing the controlled phase switching induced by the E-field in GaAs nanowires, the formation of single and multiple CPQDs. Finally, we will discuss the E-field-induced phase switching mechanisms and propose a model to explain the experimental results based on theoretical calculations and finite element simulations.

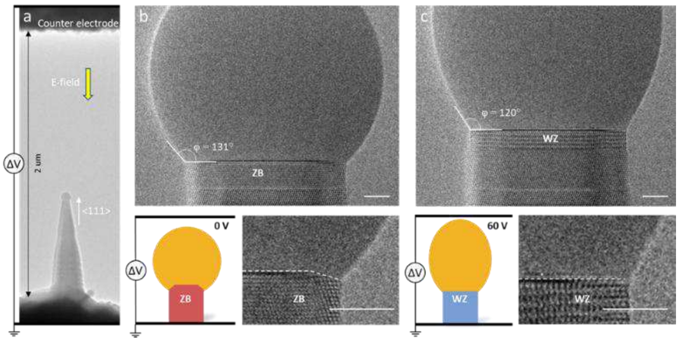

Fig.1 Crystal phase switching by electric field

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Epitaxial Growth of CaF_2 on Functionalized Si(100) Surfaces: Development of Thin Insulating Layers as a Platform for Nanoscale Device Research

E. duverger[1], D. Riedel[*2]

[1]*Institut FEMTO-ST, Univ. Bourgogne Franche-Comté, CNRS, 15B avenue des Montboucons, F-25030 Besançon, France.*

[2]*Institut des Sciences Moléculaires d'Orsay (ISMO), CNRS, Univ. Paris Sud, Université Paris-Saclay, F-91405 Orsay, France.*

*corresponding author: damien.riedel@universite-paris-saclay.fr

Mastery of silicon epitaxy is critically important across various fields, including physics [1], chemistry [2], nanoscience, microelectronics [3], and molecular electronics. As current device fabrication reaches unprecedented miniaturization (~5 nm), it has become particularly relevant to have a clear understanding and precise knowledge of the atomic structure and electronic properties of epitaxial ultra-thin films on silicon [4]. The growth of CaF_2 epitaxy is relatively well understood on a mesoscopic scale, particularly when the layer thickness is several nanometers. However, the detailed structure of ultra-thin layers, including the initial stages of epitaxy formation has remained largely unknown until now. This poster presents the evolution of our research in this area over several years, beginning with the study of CaF_2 wetting layer formation on Si(100) [5] and extending to a comprehensive characterization of CaF_2 ribbon of stripes [6]. We will also introduce the characteristics of a new, periodically spaced structure with relevant semi-insulating properties [7]. This research has benefited from top-tier theoretical support. Using density functional theory calculations, we have been able to provide numerous complementary insights into the atomic structure of these epitaxial layers as well as their insulating properties. Together, these investigations offer an appealing alternative to NaCl/Au insulating layers, enabling functionalized semi-insulating layers with surface gaps of ~ 4 eV.

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GIXRD study of epitaxial CuO films grown on SrTiO$_3$(100) by atomic oxygen assisted MBE

M. De Santis[1], V. Langlais[2], L. Martinelli[1] and X. Torrelles[3]

[1] *Institut Néel, CNRS, Université Grenoble Alpes, Grenoble INP, BP 166, 38042, Grenoble, France*

[2] *CNRS, CEMES, BP 94347, 29 rue Jeanne Marvig, F-31055, Toulouse, France*

[3] *Institut de Ciència de Materials de Barcelona, ICMAB-CSIC, Bellaterra, Barcelona 08193, Spain*

Bulk CuO has a monoclinic structure. However, thin tetragonal films (t-CuO) can be obtained by epitaxy on SrTiO$_3$(100) [1]. In this phase, the distance between (001) planes is increased compared with the NaCl structure, giving them 2D characteristics. The similarity between t-CuO electronic structure and that one of high-Tc superconductors suggests that these films could be made supra by doping. Moreover, the Cu-O-Cu bonding angle of 180° strengthen the super-exchange interaction with respect to the monoclinic phase improving the CuO magnetic properties [2].

MBE growth of CuO requires a strongly oxidant environment. Films were grown using a cracker that delivers atomic oxygen during MBE deposition of pure copper on the SrTiO$_3$ substrate held at 600 °C.

The films structure was investigated by grazing incidence x-ray diffraction performed at the European Synchrotron Radiation Facility using the dedicated In Situ Nanostructures and Surfaces (INS2) apparatus of the BM32 beamline.

Fig.1. shows a reciprocal space map of the diffracted intensity collected on a film of about 6 nm thickness, close to critical one for tetragonal to monoclinic transition. Indeed, both phases are observed. The tetragonal phase is in coherent epitaxy, as shown by the in-plane position of the t-CuO(111) peak. A ratio c/a of 1.33(2) is obtained for the lattice constants. This large tetragonal distortion agrees with a strong 2D character of the electronic structure [3].

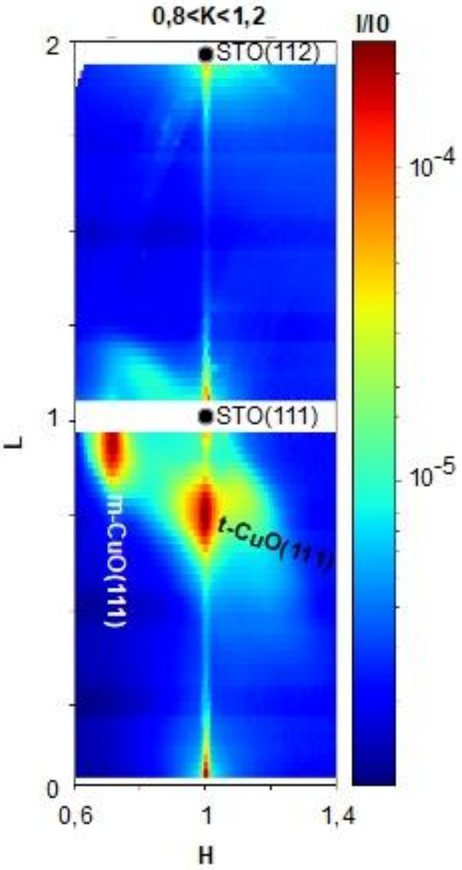

Fig. 1. GIXRD map of 6 nm CoO/SrTiO$_3$ (100)

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Grazing Incidence Fast Atom Diffraction in high-pressure conditions

H.Khemliche[1], A. Mukherjee[1,2], A. Momeni[1], E.M.S. Casagrande[1], T. Minea[3]

[1] *Institut des Sciences Moléculaires d'Orsay, Université Paris Saclay , 91400 Orsay, France*
[2] *Institut des Nanosciences de Paris, Sorbonne Université, 75005 Paris, France*
[3] *Laboratoire de Physique des Gaz et des Plasmas, Université Paris Saclay, 91405 Orsay, France*
*corresponding author : arindam@insp.jussieu.fr

Grazing Incidence Fast Atom Diffraction (GIFAD) [1] is a surface characterization technique that has been used over a decade to explore different types of materials . Here He° atoms having energy between 0.2-5 keV are scattered from the surface. The very small angle of incidence (<1°) makes the technique extremely sensitive to the topmost layer of the surface. The information derived from the diffraction data relates to the valence electron density profile of the surface atoms (electronic corrugation). The most successful application of GIFAD is to control the thin film growth of materials in a real-time in Molecular Beam Epitaxy (MBE) deposition systems.

The above description clearly shows that GIFAD is suitable for the UHV systems and all the previous work have been performed in UHV conditions. The major challenge of operating GIFAD at high-pressure ($>10^{-6}$ mbar) is the reduction of transverse coherence length as the multiple collisions broadened the beam divergence angle. At the same time high operational pressure reduces the efficiency of MCP-based detectors.

We have developed a new high-pressure GIFAD (HP-GIFAD) setup that can operate up to $\sim10^{-2}$ mbar of pressure [2]. This new development opens up the platform to study the evolution of diffraction signal at high pressure. We have found that with the increase of Ar pressure the quantum scattering from surface shifts toward to the classical scattering and decoherence phenomenon is observed. At the same time this newly developed high-pressure GIFAD is perfectly suitable to adapt in different high-pressure deposition systems such as Magnetron Sputtering (MS), Pulsed Laser Deposition (PLD), etc,. The ultimate goal will be to grow high quality thin film using High Power Impulse Magnetron Sputtering (HiPIMS), a variant of MS and control the deposition parameters in real-time using HP-GIFAD.

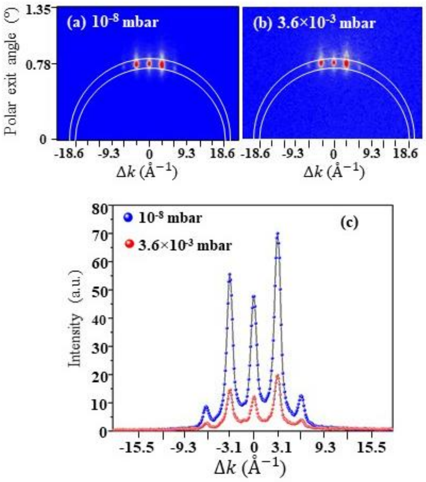

Fig. 1. (a) Diffraction images are at 10^{-8} mbar and at (b)10^{-3} mbar of Ar pressure. The projected intensities of (a) and (b) are shown in (c).

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In-Situ TEM Observation of III-V Nanowire Nucleation on Si substrate

Chen Wei,[1] Abderrahim L. Alaoui,[1] Laurent Travers,[1] Julien Chaste,[1] Cléophanie Brochard,[1] Andrea Cattoni,[1] David Bouville,[1] Etienne Herth,[1] Jean-Christophe Harmand,[1] Federico Panciera[1]

1 : Université Paris-Saclay, CNRS, Centre de Nanosciences et de Nanotechnologies, 91120, Palaiseau, France.
Corresponding author: chen.wei@c2n.upsaclay.fr

Keywords: nanowire nucleation, in-situ TEM, micro-fabrication, Raman spectroscopy

Nanoscale interfaces between heterostructures exhibit unique phenomena that differ significantly from their bulk counterparts, particularly in determining device performance and quality. The monolithic integration of silicon substrates with III-V compounds is especially promising for practical applications, as it relies heavily on the precise control of the nanoscale interface. However, the early stages of growth, which critically determine interface properties, remain poorly understood and have primarily been studied using ex-situ techniques.

In this study, we provide real-time insights into the nucleation and growth dynamics of self-catalyzed GaAs nanowires, emphasizing the formation and evolution of the nanoscale interface. Using a transmission electron microscope (TEM) equipped with molecular-beam epitaxy (MBE) sources, we monitored the interface development in situ with high spatial and temporal resolution. Custom-fabricated electron-transparent <111>-oriented Si membranes, designed via MEMS technology, served as the growth platform. The sample temperature was calibrated and optimized through finite-element simulations and Raman spectroscopy, with validation provided by the dimensions and distribution of pre-deposited Ga droplets.

Our observations revealed key processes at the interface, including Ga droplet deposition, crystal nucleation, and the early-stage lattice matching between GaAs/Si and GaP/Si. The results highlight the interplay between growth conditions and interface structure, shedding light on the mechanisms that drive heteroepitaxy. By enabling the direct epitaxy of nanowires and real-time monitoring of interface formation, this work advances the understanding of nanoscale interface dynamics and their impact on heterostructure integration.

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Nano-architecture of mixed molecular layers on a silver surface.

Yimin Guan [a], Kirill Bobrov [a], Laurent Guillemot [a]
[a] *Université Paris-Saclay, CNRS, Institut des Sciences Moléculaires d'Orsay, 91405 Orsay, France*

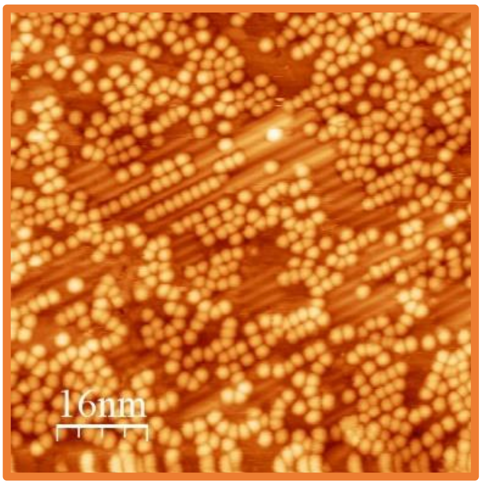
Corresponding author email: laurent.guilemot@universite-paris-saclay.fr

We present a study of the formation of mixed organic molecular layers on a Ag(110) surface.

We focus on layers of an Aromatic Polycyclic Hydrocarbon (APH) molecule, namely **perylene**, with added **fullerenes** (C_{60}). We use surface science techniques such as STM/STS, UPS/XPS and others to investigate the structure of these molecular assemblies and to study the link with their electronic, optical and vibrational properties.

We focus on these particular molecules because we demonstrated that the 3D structure of perylene multilayers on Ag(110) shows very interesting structural properties [1]. This overlayer has the unique ability to adapt to the morphology of the underlying substrate preserving its lateral order and maintaining an epitaxial relationship with the various surface terraces. Moreover, in the domain of photosynthesis perylene along with fullerene has proved to be efficient in an important process like "Triplet-Triplet Annihilation – Up Conversion" (TTA-UC) [2,3]. TTA-UC finds useful applications in OSC (Organic Solar Cells), OLED (Organic Light Emitting Diodes) and even in Photolysis cancer therapy.

We present a study on the ability of the perylene multilayer to be used as a template for forming composite layers with fullerenes (C_{60}).



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Study of Ga for Cd ion exchange under Ga gas precursor

G. HALLAIS [1*], H. MELHEM [1], G. PATRIARCHE [1], N. FINDING[1], L. LARGEAU[1], C. RENARD [1],
L. VINCENT [1]

[1] *Université Paris-Saclay, CNRS, Centre de Nanosciences et de Nanotechnologies, 91120, Palaiseau, France*

*geraldine.hallais@universite-paris-saclay.fr

When depositing a thin layer of AsGa on CdS substrate by Ultra-High Vacuum Chemical Beam Epitaxy with trimethyl gallium (TMGa) and tertiary butyl Arsine (TBAs) precursors, a ternary alloy CdGaS without As is created between the substrate and the AsGa layer.

In order to understand why and how this alloy is created and to further control its composition and thickness, a study was carried out by exposing the CdS surface only to a Ga gas precursor. For this purpose, we changed the exposure time, the type of Ga precursor (TMGa vs TriethylGallium (TEGA)) and the type of substrate (CdS vs CdSe or ZnS). Analyses of surfaces were performed before and after exposure to the Ga precursors by X-Ray Photoelectrons Spectrometry (XPS)implemented in the growth/characterisation cluster equipment so that the sample is not exposed to air. XPS shows the disappearance of the Cd from the surface along with the formation of S-Ga bonds. STEM/EDX analyses have been used to show the presence of a ternary alloys CdGaS (or CdGaSe) underneath a GaS top layer (or GaSe). The thickness and crystal structure of these layers vary depending on the type of Ga precursor and exposure time. Additional analyses in X-ray Diffraction confirm the epitaxial relationship of these layers with the substrate.

Based on the literature [1] [2], we discuss a , a diffusion mechanism enhanced by substitution of Cd by Ga that is assisted by the methyl groups of the TMGa precursor a.

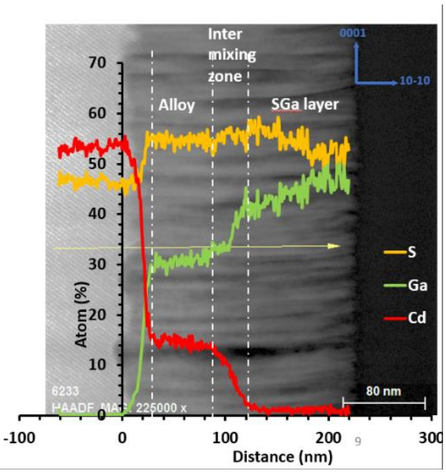

Figure 1. STEM-HAADF image with EDX profiles of a CdS susbtrate exposed during 15 min to TMGa precursor at 500°C

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Acknowledgements

Ces travaux ont été réalisés au sein des plates-formes de micro nanotechnologies C2N et soutenus en partie par le réseau RENATECH et le Conseil général de l’Essonne. Le projet de recherche est financé par le programme European Union’s Horizon 2020 research and innovation program sous la subvention 964191

(Opto Silicon). Ainsi que l’agence nationale pour la rechercher (ANR) avec le projet ANR-17-CE030–0014–01 (HEXSIGE).

Towards single molecule femtoseconde dynamics

Keke YUAN[1], Céline DABLEMONT[1], Serge CARREZ[1], Aimeric OUVRARD[1]
[1] *Institut des Sciences Moléculaires d'Orsay, Université Paris-Saclay, CNRS, 91405, Orsay, France*
*corresponding author: aimeric.ouvrard@universite-paris-saclay.fr

Understanding ultrafast optical and vibrational processes in molecules on surfaces is a key for the design and performance of organic optoelectronic devices [1]. Optical processes can be probed at the single-molecule level using scanning probe microscopy and plasmon enhanced optical spectroscopies; however, their temporal resolution is intrinsically limited [2]. In this context, we aim to go beyond the diffraction limit of optical spectroscopy and beyond the temporal response of scanning probe microscopy. We propose to combine ultrafast sum-frequency generation (SFG) spectroscopy an ideal tool to probe molecules at surfaces [3], with scanning tunneling microscopy (STM), in order to probe the vibrational dynamics of single molecules. In a similar way to tip-enhanced Raman spectroscopy, the STM tip will amplify both linear and non-linear local electric fields thanks to the localized surface plasmon resonance (LSPR).

First, we have conducted a feasibility study by numerical calculations using COMSOL, based on solving Maxwell's equations using the finite element method. In order the valid the model, we have simulated the plasmonic response of core-shell metal nanoparticles (NPs) and compared it with differential reflectance spectroscopy experiments. We were able to assign absorption bands to the NP LSPR and understand the impact of their shape and composition [4]. Then we have used the model to simulated the linear optical response of a plasmonic tip close to a surface. The electric field distribution and far field reflectivity were computed. A parametric study was conducted to estimate the impact of tip geometry, laser wavelength and polarization. Simulations demonstrate the high sensitive of the field enhancement to the tip apex radius or laser wavelength. The strongest enhancement is reached when the laser field polarization is TM, parallel to the tip long axis. A strong enhancement factor of the electric field at the sum frequency is obtained, that is large enough to overcome the small surface of emission under the tip. Experimentally, we have installed optics on the STM head in vacuum, to bring lasers and focus them at the tip apex. A high-numerical aperture lens is used to efficiently collect SFG in a plane orthogonal to the plane of incidence.

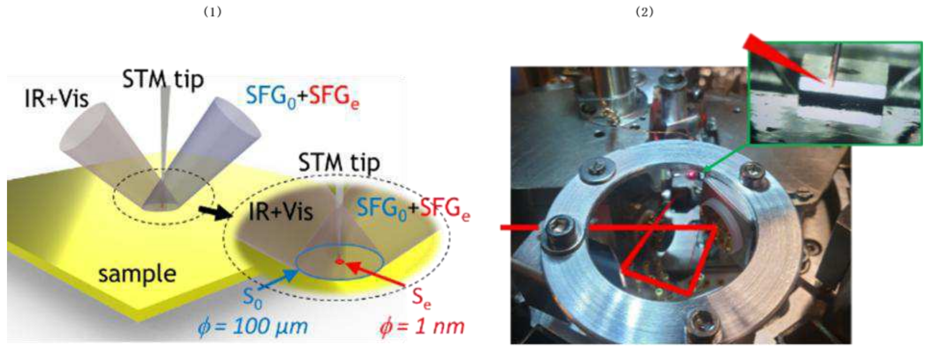

Fig.1. (1) Principle of tip-enhanced SFG and (2) experimental setup installed on the STM head

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Ultra-thin films of lead iodide on graphene: influence of the substrate on the opto-structural properties probed in real time

C.P. Sonny Tsotezem[1], A. Ouvrard[1], A. Momeni[1,2], A. Ouerghi[3], E. M. Staicu Casagrande[1] and H. Khemliche[1]

[1]*ISMO, Université Paris-Saclay, CNRS, 91405, Orsay, France*

[2]*CY Cergy Paris Université, 95000 Cergy, France*

[3]*C2N, Université Paris-Saclay, CNRS, 91405, Orsay, France*

*corresponding author: christian-perest.sonny-tsotezem@universite-paris-saclay.fr

Lead iodide (PbI_2) is a large bandgap 2D layered material belonging to the metal halide family. It has emerged as an excellent candidate for photodetectors and is a key component in metal halide perovskites solar cells. In the current work, we highlight the influence of the interface interaction on the crystalline and opto-structural properties of lead iodide layers deposited on graphene/SiC(0001) by Molecular Beam Epitaxy.

To achieve the best control of the growth process, the growing layer is characterized in real-time by GIFAD (Grazing Incidence Fast Atom Diffraction), QMS (Quadrupole Mass Spectrometry), and SDRS (Surface Differential Reflectance Spectroscopy). In particular, GIFAD provides fine information on the organization dynamics and the electron density profile at distances similar to those probed by local probes such as STM or AFM [1]. This electron density profile, which is directly related to the atomic positions within the lattice, can also be used to extract possible charge transfer within the lattice and/or with the substrate. GIFAD being a very soft technique, it can monitor the growth of the most fragile materials for hours without any damage [2]. SDRS yields information on the optical properties, which can then be correlated to the structural changes of the growing layer provided by GIFAD.

The GIFAD data reveal a layer-by-layer growth (fig. 1) by van der Waals epitaxy according to the armchair (PbI_2)/zigzag (graphene) stacking with non-commensurability of unit cells. We observe a 1.1% strain, correlated to an increase of the band gap, as well as specific optical features on the first monolayer that could result from an interface interaction stronger than van der Waals.

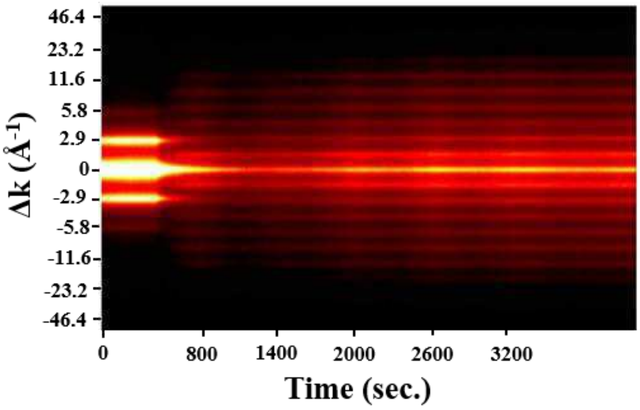

Fig. 1. Real-time monitoring by GIFAD of the growth of PbI_2 on graphene/SiC(0001). The intensity oscillations demonstrate a layer-by-layer growth, with a well-defined alignment of the lattices.

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Investigation of magnetite oxidation to maghemite via in situ XPS analysis during annealing in dry air

S. Mtakham[1], B. Domenichini[1], O. Heintz[1], H. Magnan[2], A. Barbier[2], C. Dupont[1]

[1]*Département Interfaces, ICB UMR 6303 CNRS-université de Bourogne, Dijon, France*

[2]*Service Physique Etat Condense (SPEC), CEA-Université Paris Saclay-CNRS, Gif Sur Yvette, France*

*Saida.Mtakham@u-bourgogne.fr

Among the methods used to produce hydrogen in a cheaper and, maybe, simpler way, one can mention water photolysis. This reaction corresponds to the dissociation of water molecules from sunlight energy promoted by a photocatalyst. Promising catalysts belong to transition metal oxide materials because of their stability. Among them, iron oxides appear to be very interesting thanks to their abundance in nature, their outstanding corrosion resistance and their non-toxicity even though their activity as photoelectrodes remains low. For this latter reason, we are conducting fundamental studies on the interfacial reactivity of these materials to understand the reasons for this low activity.

In this study, we have used in-situ X-ray photoelectron spectroscopy (XPS) to characterize the stability under dry air (p = 1 hPa), i.e. the oxidation of an epitaxial film (6 nm) of magnetite (Fe_3O_4, spinel structure) grown on Pt(111) single crystal. Even though the Fe2p core level is complicated to interpret when iron has mixed valences (see on Fig. 1), we succeeded in showing that this oxidation takes place in two stages, one below 100°C and a second one at 275°C. To distinguish between these two oxidation steps, Angle-resolved XPS analyses were carried out, showing that the first oxidation affects only the topmost layers, while the second impacts deeper layers. X-ray diffraction (XRD) analysis further showed that spinel structure is kept conserved during oxidation leading to maghemite phase (γ-Fe_2O_3) revealing a point defect oxidation process as in the case of nanosized magnetite particles. Besides, we have also shown that maghemite can be then reduced in magnetite when simply annealed at 400°C in vacuum, epitaxy ensuring the spinel structure stability. Many cycles of oxidation/reduction are possible.

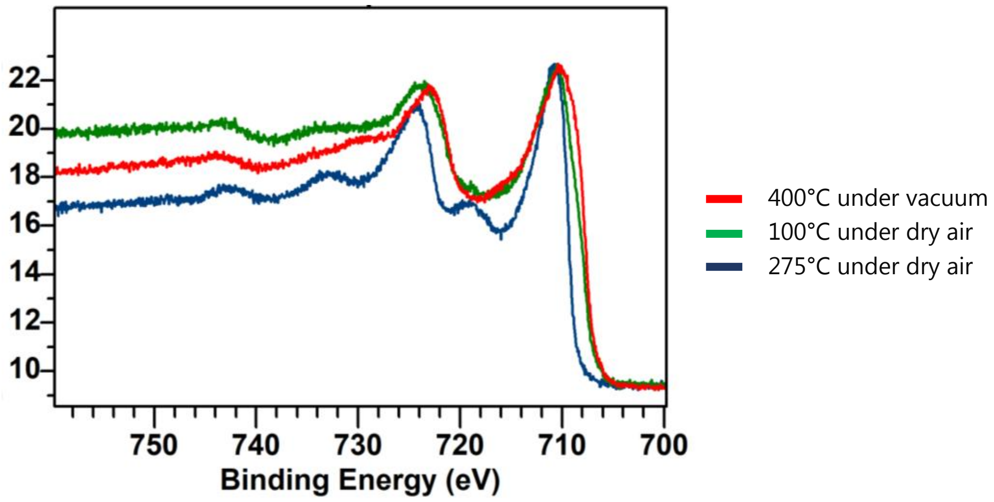

Fig.1. XPS spectra of Fe 2p core level at different stages of magnetite oxidation.

Self-Assembled $Ti_3C_2T_X$ MXene Thin Films for High-Performance Ammonia Sensors

Elmehdi Ould Maina[1,2], Elmehdi Ould Maina[1,2], Pingping Ni[2], Kassiogé Dembélé[2,3], Diana Dragoe[4], Abderrahim Yassar[2], Fatima Bouanis[1,2,*]

[1]COSYS-IMSE, Université Gustave Eiffel, F-77454 Marne-la-Vallée, France
[2]LPICM, CNRS, Ecole Polytechnique, Institut Polytechnique de Paris, 91128 Palaiseau, France
[3]Centre Interdisciplinaire de Microscopie électronique, Ecole Polytechnique, 91120 Palaiseau, France
[4]Université Paris-Saclay, ICMMO, UMR 8182 CNRS, 91405 Orsay, France

*corresponding author: fatima.bouanis@polytechnique.edu.

MXenes have emerged as a fascinating material for RT gas-sensing applications due to their outstanding properties. This work reports the design and fabrication of a high-performance ammonia sensor based on MXenes material. To improve its sensing performance, a MXenes nanosheets thin film with a thickness of ≈ 10 nm was prepared using a scalable self-assembled method. Specifically, we employed the controlled and enhanced interfacial self-assembled method to fabricate a continuous and conductive MXene ultra-thin film. The morphology and the structure of the produced MXene materials and their films were characterized by combining multi-characterization tools. Altogether, these highlight the uniform and continuous deposition of the MXene nanosheets film on the glass substrate. The electrical characterization indicates a sheet resistance value of 4.82×10^5 Ω/sq. The fabricated devices present good RT sensing performances for NH_3 detection, ranging from 1 to 20 ppm. This demonstrates the outstanding sensitivity of MXene with a value of 1.92 % for the lowest concentration (1 ppm), a fast response (179 s) and a recovery time of (612 s), which is related to the high quality of the ultra-thin MXene sensiting layer. [1] Moreover, the sensors demonstrate high degree of stability and excellent reproducibility, make them suitable candidate for practical applications like environmental monitoring.

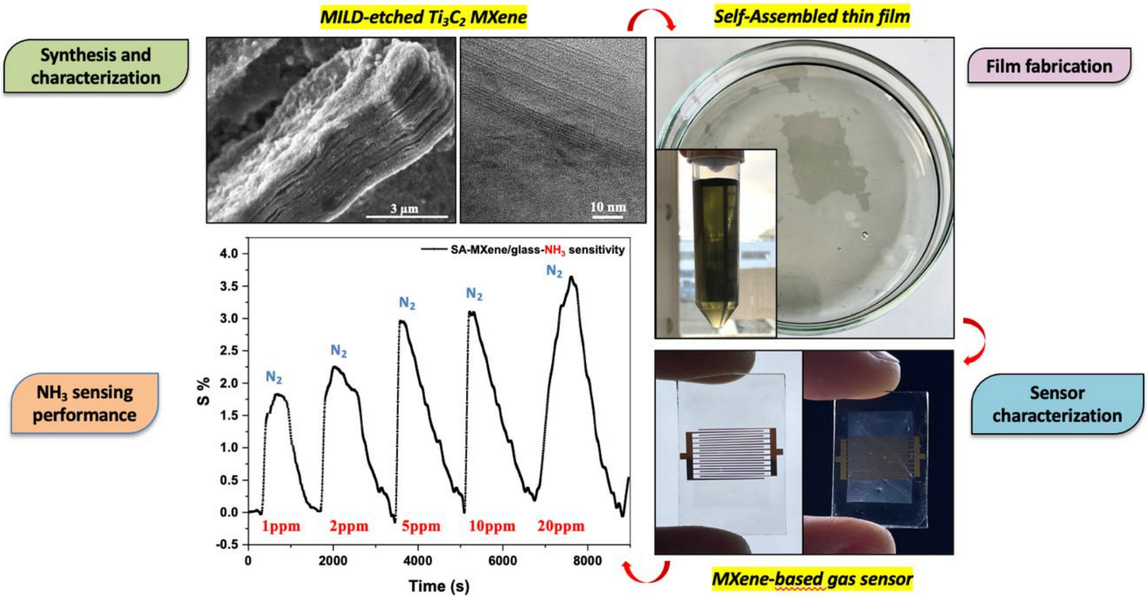

Figure 1: (a) SEM and TEM image of Ti_3C_2 MXene. (b) MXene colloidal solution (inset) and Interfacial self-assembled film. (c) Typical MXene based gas sensor. (d) Gas sensors response to 1-20 ppm NH_3.

[1] **E. Ould Maina et al.,** Self-Assembled $Ti_3C_2T_X$ Mxene Thin Films for High-Performance Ammonia Sensors. *Applied Surface Science* 2024, 672, 160864.

Interfacial self-assembly between polydiacetylene and graphene oxide

Alexia Bistintzanos[1], S. Spagnoli[1], H. Cruguel[1], Y. Prado[1], P. Fontaine[2], A. Hemmerle[2], F. Carlà[3],M. Goldmann[1,2]
[1]*Institute of Nanosciences of Paris, UMR 7588, CNRS, Sorbonne University, 75005 Paris, France*
[2]*Synchrotron SOLEIL, 91190 Saint-Aubin, France*
[3]*Synchrotron Diamond Light Source, Oxfordshire, OX11 0DE, United Kingdom.*
alexia.bistintzanos@insp.jussieu.fr

This study ultimately seeks to form and study the interface between a polydiacetylene (PDA) and graphene oxide (GO). The reason is that a multi-layered structure based on these two compounds features promising optoelectronic applications [1], such as solar photovoltaic (Fig.1). However, the interesting and exploitable optical and conductive properties of this hybrid system rely on the organization between GO and PDA at the interface. Hence, there is a need to obtain and understand such an interface. The Langmuir procedure is used to form the interfacial assembly on a liquid subphase. GO sheets and diacetylene (DA) monomers are deposited on a water surface. Their amphiphilic properties make them stay on the surface of the water and not sink. The two species are compressed, and, eventually, one is expected to climb over the other one, forming the interface. Then, the diacetylene monomers are polymerized to obtain the desired assembly of GO and PDA. The polymerization occurs when the diacetylene molecules are exposed to UV or X-ray irradiation. First, the mixed GO/DA system is studied directly on the liquid subphase (before polymerization) by Π-A isotherms, Brewster Angle Microscopy (BAM), and X-ray scattering techniques; in particular Grazing Incidence Diffraction (GIXD) and Reflectivity (XRR) using a synchrotron source. Then, after polymerization, the optical properties of the hybrid film are examined by UV-vis absorption. Eventually, the GO/PDA mixed film is transferred onto a solid substrate for Atomic Force Microscopy (AFM), Kelvin Probe Force Microscopy (KPFM), RAMAN, and X-ray Photoelectron Spectroscopy (XPS) measurements.

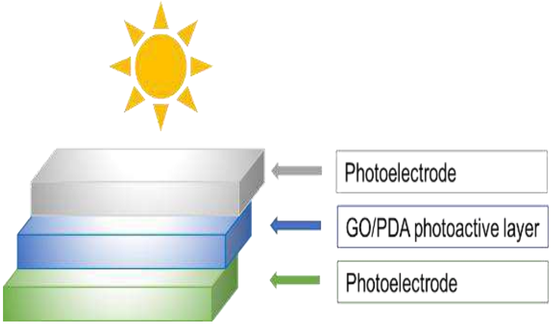

Fig.1. Schematic representation of an organic solar cell with a GO/PDA interface as the photoactive layer

[1] E. A. Gusarova et al., Colloid and Interface Science Communications **46**, 100575 (2022).

Langmuir-Blodgett monolayers: a joint study by femtosecond vibrational spectroscopy and Grazing Incidence X-ray Diffraction

Léa-Marion Lin[1], A. Hemmerle[2], P. Fontaine[2], A. Ouvrard[1], S. Carrez[1], W. Zheng[1],
C. Dablemont[1,*]
[1]*ISMO, Université Paris-Saclay, CNRS, 91405, Orsay, France*
[2]*Synchrotron SOLEIL, L'Orme des Merisiers, 91192, Gif sur Yvette, France*
*corresponding author: celine.dablemont@universite-paris-saclay.fr

Langmuir-Blodgett (LB) films [1] find practical applications in electronics [2], optics, applied chemistry, micromechanics, biology and medicine [3] etc. Over the past 30 years, crystalline properties of various LB MonoLayers (ML) have been well-characterized before transfer, on the water subphase, using Grazing Incidence X-ray Diffraction (GIXD). Vibrational Sum Frequency Generation (SFG) is surface sensitive non-linear optical spectroscopy method from which the vibrational modes of methyl CH_3 groups provide information on the molecular orientation and conformational structure [4]. This study attempted to compare the tilt angle θ of the C backbone values obtained from GIXD and SFG. Suitable data have been collected on a ML of the DPPC (1,2-dipalmitoylphosphatidylicholine) phospholipid by polarization-resolved SFG (left part of Fig.) on glass. The tilt angle has been measured on series ($H_3C\text{-}(CH_2)_n\text{-}COOH$ n=16 stearic, n=19 heicosanoic and n=20 behenic) of carboxylic acids by GIXD on silicon substrates (right part of Fig.). Trying to improve the signal-to-noise ratio in GIXD on glass substrates by increasing the signal and decreasing the X-ray penetration in the substrate, we proposed an experimental method to vary the tilt in the third layer of a trilayer and measured on glass the phospholipid DPPS (1,2-dipalmitoyl-sn-glycero-3-phosphoserine) layers. In this topic, one objective is to address the remaining disagreements about transfer effects [5].

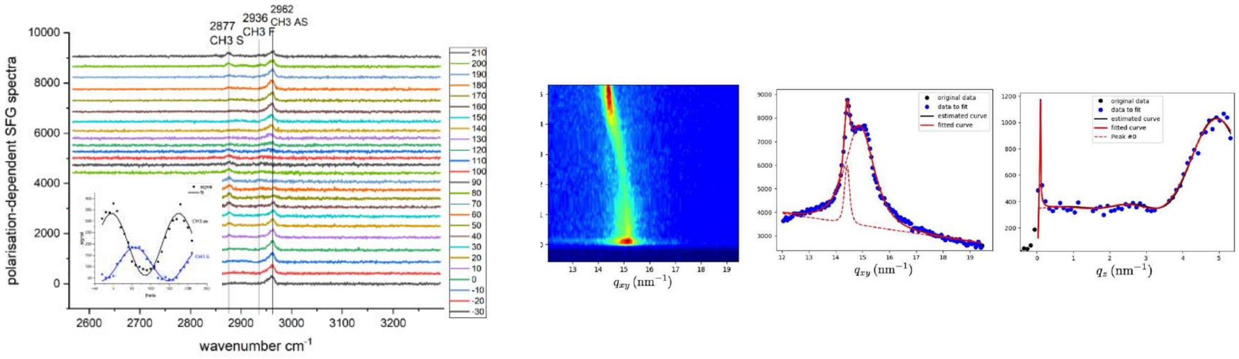

Fig. (Left) DPPC ML on glass at 20 mN/m: polarization-dependent SFG spectra and, in the inset, experimental evolution of the intensity with respect to the polarization angle and fit. (Right) GIXD spectrum of behenic acid deposited on silicon at 20 mN/m, and associated fits of the peaks along qxy and qz. Analysis of the positions of the peaks led to a tilt angle of 22°.

[1] M. Gabaji, J. Médard, A. Hemmerle, J. Pinson, J.-P. Michel, Langmuir **36**, 2534-2542 (2020).
[2] M. Singh, N. Kaur, E. Comini, J. Mater. Chem. C **8**, 3938-3955 (2020).
[3] D. Samantha, A. Sarkar, Chem. Soc. Rev. **40**, 2567-2592 (2011).
[4] Z. Guo et al, Surf. Sci. **602**, 3551-3559 (2008).
[5] D. W. Schwartz, Surf. Sci. Rep. **27**, 245-334 (1997).

Study and Characterization of TzDA Langmuir Films for Polydiacetylene-Based Sensors

Kandyli Maria[1,2], Sylvie Spagnoli[1], Hayfa Jeridi[2] and Michel Goldmann[1], Philippe Fontaine[3], Arnaud Hemmerle[3], Hervé Cruguel[1].
[1]*Institute of Nano-Sciences of Paris (INSP), Sorbonne University, Paris, France*
[2]*Laboratory of Research in Interdisciplinary Digital Engineering & Sciences (LyRIDS), ECE Engineering School, Paris, France*
[3] *Synchrotron SOLEIL, L'Orme des Merisiers, Saint Aubin, BP48, 91192 Gif sur Yvette Cedex, France*
*corresponding author: mkandyli@ece.fr

Diacetylenes polymerize under irradiation to form blue polydiacetylenes (PDAs), known for chromogenic and fluorogenic transitions.[1] Conversion of blue to red PDA occurs under various stimuli, but the red form's low fluorescence limits sensitivity. To improve this, we propose TzDA, a di-alkyl backbone molecule modified with a tetrazine fluorophore to enhance fluorescence recovery.[2] Our goal is to develop ultra-thin, sensitive sensors using homogeneous and polymerizable TzDA Langmuir films (Fig. 1).

The Langmuir technique creates monomolecular films by spreading amphiphilic molecules in a volatile solvent on a water/air interface. After solvent evaporation, barriers compress the film, and surface pressure (Π) vs. area per molecule (Apm) is measured, revealing 2D phase transitions.

Under UV irradiation, TzDA Langmuir films undergo polymerization, yielding a blue-phase polymer. Notably, the initial results presented here pertain specifically to the unpolymerized monomeric film. Initial experiments showed unusual Π-Apm isotherms: as temperature dropped from 20°C to 5°C, the lift-off point (area at which surface pressure begins to rise, indicating full surface coverage) shifted to higher areas without any detectable 2D phase transitions. Brewster Angle Microscopy (BAM) confirmed no phase transitions, indicating a condensed phase. Atomic Force Microscopy (AFM) analysis of films transferred onto solid substrates revealed the coexistence of monolayer and multilayer domains, with measured thicknesses indicating a tilted molecular conformation. Grazing Incidence X-ray Diffraction (GIXD) showed no signal from monolayer domains, but a well-ordered, tilted (45°) structure in multilayer regions. X-Ray Reflectivity (XRR) confirmed an average film thickness compatible with mixed mono- and multilayer structures.

UV-Vis spectroscopy of irradiated films showed decreased absorbance at lower temperatures, likely due to enhanced molecular spreading, suggesting reduced multilayer formation. These findings indicate TzDA rapidly forms multilayered films at low surface pressures, where only well-ordered domains contribute to polymerization.

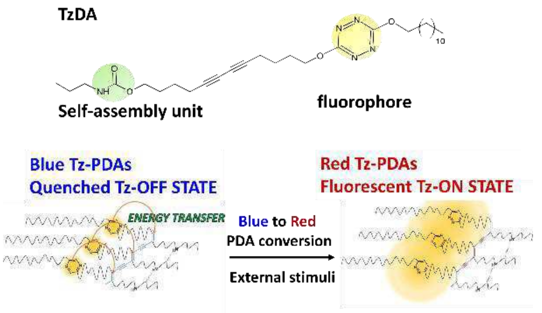

Figure 1 : Structure of TzDA and scheme of fluorescence signal modulation according to the PDA state.

[1] F. Fang, F. Meng, and L. Luo, "Recent advances on polydiacetylene-based smart materials for biomedical applications," Mater. Chem. Front., vol. 4, pp. 1089‑1104, 2020.

[2] X. Qian and B. Städler, “Recent developments in polydiacetylene-based sensors,” Chemistry of Materials, vol. 31, no. 4, pp. 1196–1222, 2019.

Magnetic skyrmions in ultrathin films

Stanislas ROHART[1], Sujit Panigrahy[1], Sougata Mallick, Greis Cipi[1]
[1]*Laboratoire de Physique des Solides, Université Paris-Saclay*
*stanislas.rohart@universite-paris-saclay.fr

Skyrmions in magnetic layers are magnetic textures for with topology plays a crucial role and that can behave as solitons. They consist of localized spin textures that cover the entire spin unit sphere, resulting in non-trivial topology. This significantly impacts their dynamics, for instance, leading to increased dissipation at smaller sizes and a gyrotropic force that causes their trajectory to deviate from the direction of the applied force.

In this presentation, we present our recent advances in this physics. We show how they can be stabilized in magnetic multilayers by tunning, via the thickness of the magnetic layers, the micromagnetic energies (magnetic anisotropy, dipolar couplings, Dzyaloshinskii-Moriya interaction). In particular, we show how it is possible to stabilized true solitonic skyrmions at zero applied magnetic field. We also show the manipulation using electrical current and discuss the relevant underlying mechanisms to reach a high efficiency. The dynamics show furthermore a gyrotropic deflection with a deflection away from the applied current direction, which arises from the skyrmion topology (fig. 1a). In a second part, we present our results on synthetic antiferromagnetic skyrmions (two magnetic layers antiferromagnetically coupled via a non-magnetic spacer). These experiments show that, by coupling two magnetic skyrmions with opposite topology, the gyrotropic deflection can be suppressed and the velocities can be increased (fig 1b).

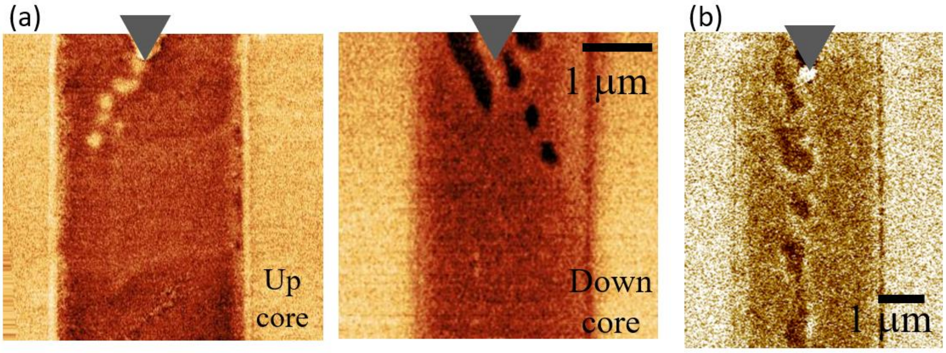

Fig.1. Magnetic motion of skyrmions in nanotracks induced by an electric current (from top to bottom). Skyrmions are nucleated at the gray triangle where the current is concentrated. In (a), the ferromagnetic skyrmions show a deflection related to there topology, and that therefore depend on their core orientation. In (b) the synthetic antiferromagnetic skyrmions, the deflection is compensated.

[1] S. Mallick et al. Phys. Rev. Appl. 18 064072 (2022)
[2] S Panigrahy et al. Phys. Rev. B 106, 144405 (2022)
[3] S. Panigrahy et al. *in preparation*

Characterization of the Electrical Properties of 2D Materials via Atomic Force Microscopy

Andrea Cerreta[1], Alexander Klasen[1]
[1] *Park Systems Europe GmbH, Mannheim, 68199, Germany*
*corresponding author: acerreta@parksystems.com

Two dimensional materials are the focus of intensive research due to the novel physical properties they manifest and their potential utilization in nano scaled electronic devices. Among others, transition metal dichalcogenides (TMD) like MoS_2 have been investigated to produce single layer transistors [1]. Moreover, TMD layered homostructures have shown to possess a ferroelectric behaviour [2] and the same applies to hexagonal boron nitride stacks [3]. The key ingredient to allow these 2D systems to show ferroelectricity is the relative twist between layers, which gives rise to superlattices where position dependent out-of-plane net polarization can be observed. The tunability of the electrical properties of twisted bilayer graphene has been also demonstrated on rotatable devices of micrometric lateral scale [4].

In order to properly get an insight into the physics of such an incredibly rich ensemble of materials and structures, it is necessary to use instruments which are able to detect the fine modulation of their electrical features with an adequate lateral resolution.

Atomic Force Microscopy (AFM) is a versatile technique to study the properties of materials at interfaces. Being introduced to obtain high resolution maps of the surface topography on the most different samples, it has proven to be able to provide much more than that. In fact, the AFM probe is sensitive to all a range of forces of different nature from which electrical, magnetic, and mechanical information about the underlying samples can be assessed.

In this talk, it will be shown how Conductive AFM to map the sample conductivity, Kelvin Probe Force Microscopy (KPFM) to study the local surface potential, and Piezoelectric Force Microscopy to understand the piezo/ferroelectric behaviour of materials can be used to visualize moiré patterns in 2D layered structures, and examples of the application of these AFM modes to the characterization of systems such as twisted hexagonal boron nitride and twisted graphene bilayers will be given.

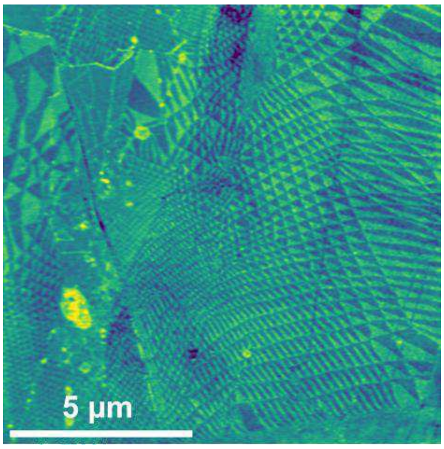

Fig.1. KPFM map of a double layer of hexagonal boron nitride showing triangular ferroelectric domains.

[1] B. Radisavljevic et al., Nat. Nanotechnol. 6, 147-150 (2011)
[2] X. Wang et al., Nat. Nanotechnol. 17, 367–371 (2022)
[3] C. R. Woods et al., Nat. Commun. 12, 347 (2021)
[4] R. Ribeiro-Palau et al, Science 361, 690-693 (2018)

Conception of a new electron microscope for surface science

Florent Vallée[1], L. Amiaud[2], N. Barrett[3], D. Compart[1]
[1]*Laboratory Aimé Cotton, University of Paris Saclay, Orsay, France*
[2]*ISMO, University of Paris Saclay, Orsay, France*
[3]*SPEC, CEA, Orsay France*
*florent.vallee@universite-paris-saclay.fr

By combining a monochromatic electrons source with high performance detectors, we build with the laboratories ISMO and SPEC a unique electronic microscope call HREELM. This microscope is able to make spatial imagery and analyse the surface vibrations interactions simultaneously. Applications include nanophysics, nanochemistry and photonics.

One of the most important things for HREELM is the electron source. The flux must be higher than 100 pA and the energy dispersion must be lower than 10 meV to be able to resolve phonons, plasmons, etc... To satisfy these criteria, we choose the Rydberg atom ionization. We use a caesium jet and three lasers to excite the atoms into a Rydberg state. Centrally drilled electrodes are used to impose an electric field on the Rydberg atoms.

The manipulation and the detection of the electrons after the sample interaction is also crucial and requires special attention. The electron energy loss spectra will be given by a time-of-flight measurement. For this reason, we need to use a special sensor who is able to measure the position and the time of arrival of the electron.

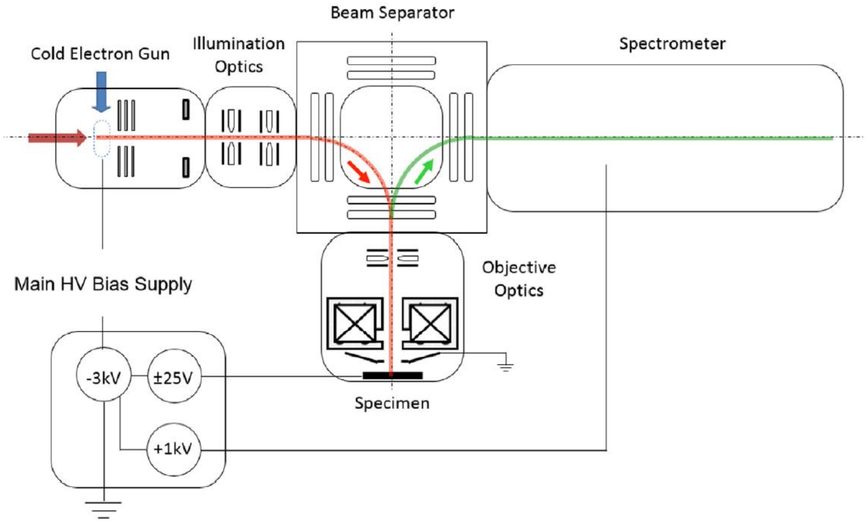

Fig.1. Final HREELM version scheme.

[1] High repetition rate sub-ns electron pulses from resonant pulsed Rydberg field-ionization R.Hahn, D.Comparat: https://arxiv.org/abs/2308.15333

[2] Cesium Rydberg-state ionization study by three dimensional ion-electron correlation : Toward monochromatic electron source R.Hahn, D.Comparat DOI : 10.1103/PhysRevA.103.042821

Control of large-area 2D crystals-noble metals interaction via interfacial alloying

Hulerich Camel Tchouekem [1], Julien Morin [1], Bruno Lépine [1], Alain Moréac [1], Mahault Berset[2], Claude Monney [2], Phillipe Schieffer [1], Jean-Christophe Le Breton [1] and Thomas Jaouen[1]

[1] *Univ Rennes, CNRS, (IPR Institut de Physique de Rennes) -UMR 6251, F-35000 Rennes, France*

[2] *Département de Physique and Fribourg Center for Nanomaterials, Université de Fribourg, CH-1700 Fribourg, Switzerland*

The exfoliation of two-dimensional (2D) layered materials such as transition metal dichalcogenides (TMDs) on noble metals (Au, Ag, Pd, Pt, ...) has recently received particular attention from the scientific community [1]. This is due to the possibility of controlling the strong quasi-covalent interaction between the first TMD layer and the metal substrate, which leads to predominant exfoliation of single layers of large lateral dimensions only limited by the quality of its layered bulk parent compound. This method has been demonstrated to produce macroscopic monolayers for more than 40 different layered materials [2], opening up a new arena for exploring the properties of emergent families of ultrathin semiconductors, metals, superconductors, topological insulators, ferroelectrics, etc., as well as engineered van der Waals heterostructures.

In this communication, we present ARPES, Raman and photoluminescence (PL) measurements performed on MoS_2 monolayer exfoliated on Au. After highlighting the strong impact of the Au substrate on the MoS_2 electronic band structure and vibrational properties, we explore the possibility of weakening the covalent-like quasi bonding at the TMD-Au interface by controlling the formation of an intermetallic alloy with an Al adhesion layer and annealing procedure [Figure 1, left-hand side]. By focusing on the evolution of two Raman modes giving spectroscopic hints on both the strain state and charge transfer at the interface as well as on PL changes [Figure 1, right-hand side], we show that annealing leads to both Raman and PL signatures characteristic of an unsupported MoS_2 monolayer. We propose that the thermally-activated Al diffusion into Au up to the MoS_2/Au interface allows for the oxidation of the as-formed Au-Al intermetallic alloy resulting in an almost complete decoupling of the MoS_2 monolayer from its metallic substrate.

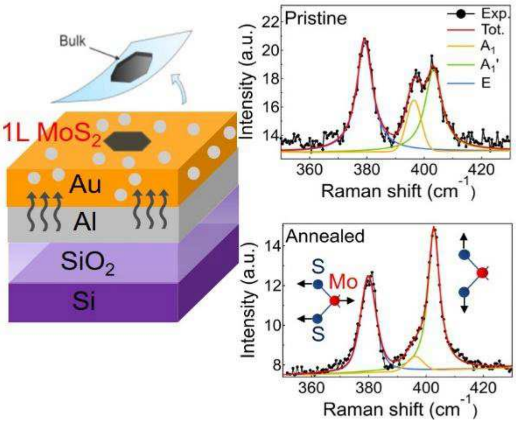

Figure 1. Left-hand side: Schematic drawing of the used experimental procedure for decoupling a large-area TMD monolayer that was exfoliated on Au. Right-hand side: Raman spectra of MoS_2 monolayer supported on Au before (pristine) and after annealing (annealed).

[1] M. Velický, G. E. Donnelly, W. R. Hendren *et al.*, ACS Nano **12**, 10463 (2018).

[2] Y. Huang *et al.*, Nat. Commun. **11**, 2453 (2020).

Controlling the luminescence of 2D materials using an STM

R. J. Peña Román[1], R. Bretel[2], D. Pommier[2], E. Boer-Duchemin[2], G. Dujardin[2], A. Borissov[2],
L. F. Zagonel[1], G. Schull[3], S. Berciaud[3], and E. Le Moal[2]
[1]*Institute of Physics “Gleb Wataghin”, State University of Campinas, Brazil*
[2]*Université Paris-Saclay, CNRS, Institut des Sciences Moléculaires d’Orsay, Orsay, France*
[3]*Institut de Physique et Chimie des Matériaux de Strasbourg, Université de Strasbourg, CNRS, Strasbourg, France*
*corresponding author: eric.le-moal@universite-paris-saclay.fr

A scanning tunneling microscope (STM) is used to electrically activate the luminescence of two-dimensional (2D) materials under the STM tip, in order to spatially resolve the variations of the excitation quantum efficiency at the nanoscale. An optical microscope and an optical spectrometer are used to spatially, angularly and spectrally resolve the emitted light, in order to study the emission processes and to identify the excitonic species involved (see Fig. 1a-c). In this way, we demonstrated the STM-induced generation of neutral and charged excitons in monolayer transition metal dichalcogenides ($MoSe_2$ and WS_2) [1,2]. Recently, we showed that the STM tip and tunneling current can also be used to control photoluminescence quantum yields in 2D semiconductors (see Fig. 1d,e) [3].

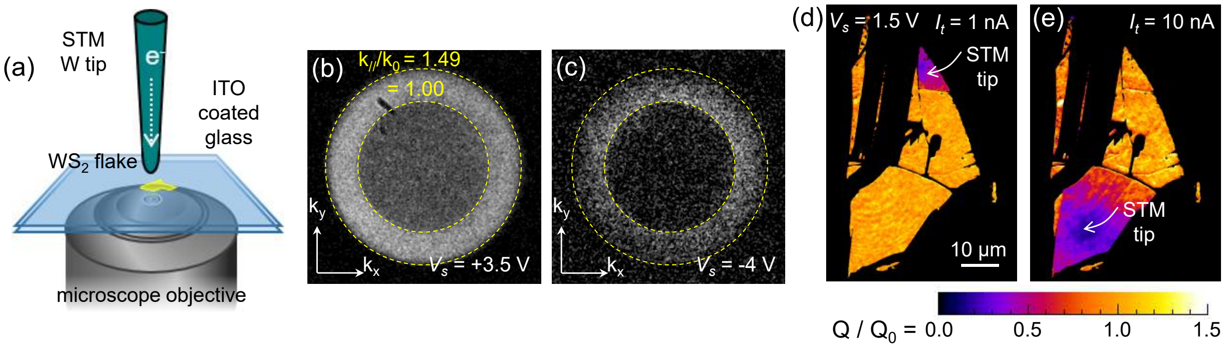

Figure 1: (a) Schematic of the experiment, showing the STM tip and the optical microscope objective. (b,c) Angular distribution of STM-induced luminescence of a WS_2 monolayer at positive and negative sample bias, respectively [2]. (d,e) False-color optical microscopy images showing the STM-controlled modification of the photoluminescence quantum yield (Q) of a WS_2 monolayer. [3].

[1] D. Pommier, R. Bretel, L. E. Parra López, F. Fabre, A. Mayne, E. Boer-Duchemin, G. Dujardin, G. Schull, S. Berciaud, E. Le Moal. *Scanning tunneling microscope-induced excitonic luminescence of a two-dimensional semiconductor*. Physical Review Letters **123**, 027402 (2019).

[2] R. J. Peña Román, D. Pommier, R. Bretel, L. E. Parra López, E. Lorchat, J. Chaste, A. Ouerghi, S. Le Moal, E. Boer-Duchemin, G. Dujardin, A.G. Borisov, L.F. Zagonel, G. Schull, S. Berciaud, E. Le Moal. *Electroluminescence of monolayer WS_2 in a scanning tunneling microscope: Effect of bias polarity on spectral and angular distribution of emitted light*. Physical Review B **106**, 085419 (2022).

[3] R. J. Peña Román, R. Bretel, D. Pommier, L. E. Parra López, E. Lorchat, E. Boer-Duchemin, G. Dujardin, A. G. Borisov, L. F. Zagonel, G. Schull, S. Berciaud, E. Le Moal. *Tip-induced and electrical control of the photoluminescence yield of monolayer WS_2*. Nano Letters **22**(23), 9244–9251 (2022).

Diffraction of fast heavy noble gas, Ne, Ar, Kr Xe, on a LiF(001) surface.

M. Debiossac[1,2], P. Pan[1], J. N. Rad, C. Kanitz[1,2] and P. Roncin[1]
[1]*Institut des Sciences Moléculaires d'Orsay (ISMO), CNRS-Université Paris-Saclay, Orsay, France*
[2]*German Aerospace Center (DLR), Inst. of Quantum Tech., Wilhelm-Runge-Str 10, Ulm, Germany*

In its principle atom diffraction at surfaces is an AFM operating in the momentum space with a perfectly defined single atom tip. We look here at the influence of the tip. Increasing its mass reduces the associated wavelength λ and the expected resolution, however, the probability to bounce on the surface without exciting phonons reduces. Also, with an increasing number of valence electrons, the Pauli repulsion becomes larger pushing the turning point further away from the surface.

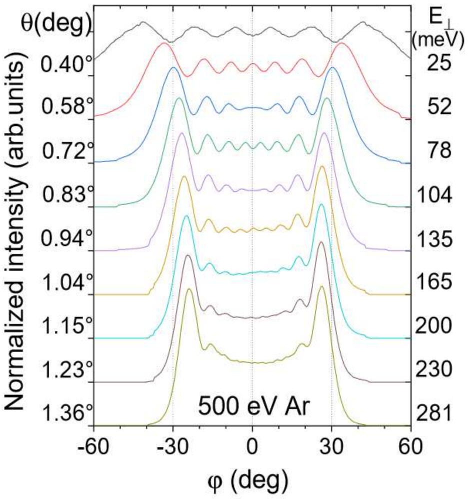

Fig.1. Azimuthal scattering profiles of 500 eV Ar along the [110] direction at various incidence angles.

With fast atoms at grazing incidence (GIFAD [1]) the projectile deflection is distributed on several successive sites providing a strong decoupling of the fast motion parallel to the surface from the much slower one in the perpendicular plane. This results in a significant reduction of the Debye-Waller factor which allows operation with heavy atoms and/or at high temperatures [2] (*e.g.* at more than 600°C on GaAs). With neon, the fraction of elastic diffraction was large enough to allow the derivation of a detailed potential energy landscape [3,4] with help of a quantum scattering code (Coll. A.G. Borisov). With argon, the elastic component is very weak but we resolve the inelastic diffraction peaks [5] at low values of $E_\perp$. while the peak overlap become important above. The qualitative and quantitative aspects of diffraction are however still present. The scattering profiles presented in Fig 1 show characteristic oscillations of diffraction. The maxima located at the highest deviation angles correspond to the “classical” rainbow while those at the smallest angles named supernumerary rainbows result from interferences between the different paths leading to the same final angle. Each maximum indicates a phase difference multiple of 2π. These oscillations are in practice the envelope describing the discrete intensities of the unresolved diffraction orders and contain all the quantum information (in the semi-classical regime). With Kr, we no longer observe an elastic component but the supernumerary rainbows remain visible. With Xe, even the supernumerary rainbows become hardly visible reducing the accuracy of the comparison with a model of potential energy landscape. The full comparison is not yet completed but the influence of the attractive forces to the surface and of the coherence length of the surface will be discussed with optical diffraction and refraction models [1,3] as well as semi-classical model [6].

[1] *e.g.* M.Debiossac, Pan & Roncin (Review comparing GIFAD with thermal energies) PCCP p7615 (2021)
[2] P.Pan *et al* “Temperature dependence in fast-atom diffraction at surfaces “. PCCP p12319 (2022)
[3] M.Debiossac, P.Roncin & A.G.Borisov « Refraction of fast Ne atoms » J. Phys. Chem. Lett. p4564 (2020)
[4] M. Debiossac *et al* “Elastic and inelastic diffraction of fast neon atoms on LiF …“. PCCP p30966 (2022)
[5] P.Pan *et al* “Lateral line profiles in fast-atom diffraction at surfaces.” Phys. Rev. B. 035413 (2023)
[6]. E. Pollak *et al* “ GIFAD…semiclassical perturbation theory .” … PCCP p25501 (2024)

Doping tunable charge density waves in misfit layer compounds

Hugo Le Du[1], Ludovica Zullo[1], Justine Cordiez[2], François Debontridder[1], Marie Hervé[1],
Laurent Cario[2] and Tristan Cren[1]

[1] *Institut des Nanosciences de Paris, Sorbonne Université, Paris, France*
[2] *Institut des Matériaux de Nantes, Nantes Université, Nantes, France*
*corresponding author: hugo.ledu@insp.jussieu.fr

Transition metal dichalcogenides (TMDs) are a class of two-dimensional materials with unique electronic, optical, and mechanical properties, making them promising for applications in electronics, optoelectronics, and related fields [1]. In particular, $NbSe_2$ exhibits both superconductivity and charge density waves, leading to an intriguing interplay between these two electronic phenomena. Misfit layer compounds are van der Waals layered heterostructures formed by stacking layers of transition metal dichalcogenides with layers of monochalcogenides. Theoretically, it has been shown that a charge transfer occurs from the monochalcogenide layers to the TMD layers, resulting in significant doping of these layers [2]. By adjusting the chemical composition of the monochalcogenide layers it is possible to tune the doping level. In particular in $(La_xPb_{1-x}Se)_{1,14}(NbSe_2)_2$, the Fermi level of $NbSe_2$ can be tuned from 0.0 eV to 0.3 eV by adjusting the x value in the chemical formula. Here, we demonstrate through density functional theory calculations and scanning tunneling microscopy measurements that $NbSe_2$ undergoes a transition from the conventional 3×3 charge density wave at low doping to a 2×2 charge density wave at higher doping, corresponding to a Fermi level shift of 0.13 eV. The superconducting critical temperature also varies with the shift of the Fermi level, offering a novel platform to explore the interplay between superconductivity and charge density waves in these materials.

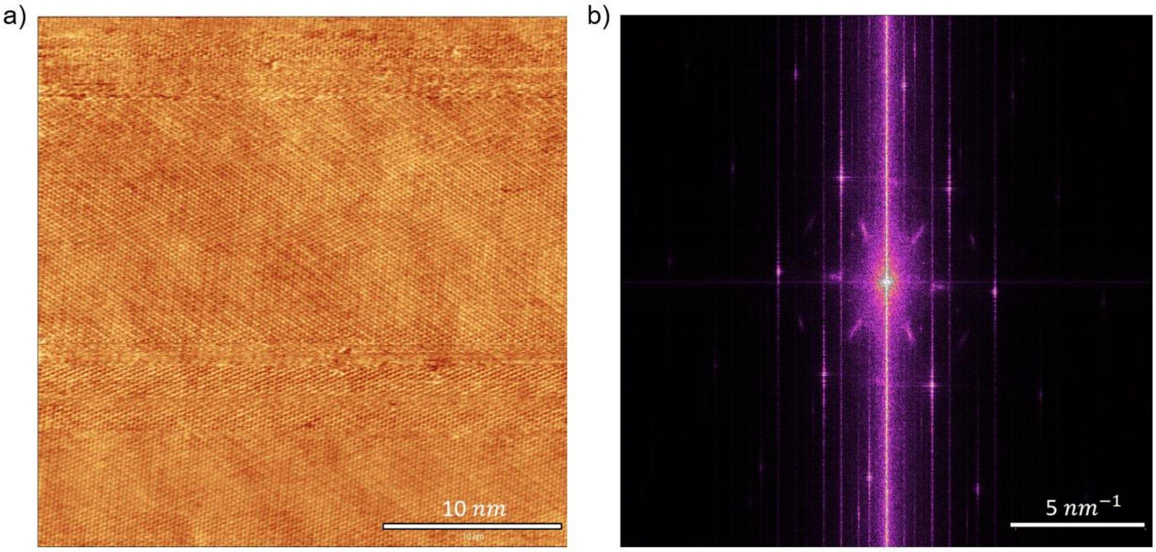

Fig. 1. a) STM image of $(La_{0.4}Pb_{0.6}Se)_{1,14}(NbSe_2)_2$ b) Associated Fourier transform exhibiting 2x2 CDW

[1] S. Manzeli et al., 2D transition metal dichalcogenides, Nature Reviews Materials 2, 17033 (2017).

[2] L. Zullo et al., Misfit Layer Compounds as Ultratunable Field Effect Transistors: From Charge Transfer Control to Emergent Superconductivity, Nanoletters 23, 14 (2023)

Electronic control of two-dimensional semiconductor photoluminescence on the nanoscale

Élysé Laurent[1], Elizabeth Boer-Duchemin[1], Séverine Le Moal[1], Guillaume Schull[2], Stéphane Berciaud[2], Éric Le Moal[1]
[1]*Institute of Molecular Sciences of Orsay (ISMO), University of Paris-Saclay, Orsay, France*
[2]*Institute of Materials Physics and Chemistry of Strasbourg (IPCMS), University of Strasbourg, Strasbourg, France*
*elyse.laurent@universite-paris-saclay.fr

Semiconductor transition metal dichalcogenides (TMD) are receiving significant attention in the field of optoelectronics due to their optical properties. Even at room temperature, the luminescence of monolayer TMDs is governed by the dynamics of their exciton, i.e., the electron-hole pairs bound by the Coulomb interaction. Previous work has shown that it is possible to monitor in real space the effects of locally injected charges carriers [1, 2], which is key for future TMD-based light emitting microdevices. Here, we introduce a new technique that makes it possible to monitor in real space the effects of locally injected charge carriers on the radiative quantum efficiency of TMDs, which was not possible using the techniques reported until now. In our technique, the wide-field laser-induced photoluminescence (PL) microscopy image of molybdenum diselenide ($MoSe_2$) monolayers is captured while charge carriers are injected into the monolayers via electron tunneling from (or to) the tip of a scanning tunneling microscope (STM). By looking the PL intensity quantum yield near the injection point located in the center of the blue circle in the PL images below, we found that the local electron injection induces long-range quenching of $MoSe_2$ PL on a micrometer size area while hole injection enhanced the PL response of the $MoSe_2$. These effects are reversible and the initial value of the $MoSe_2$ radiative quantum efficiency is recovered on a timescale of a few seconds after cutting the tunneling current. We show that the characteristic time of this recovery process depends on the laser power used to excite the $MoSe_2$ monolayers. Moreover, we present a model aim at understanding the spatial variation of the observed quenching phenomenon.

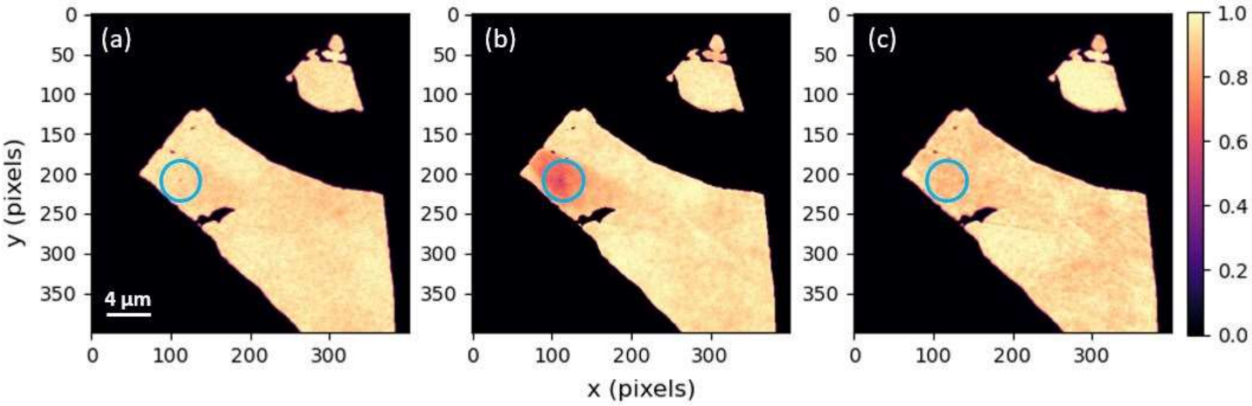

Fig.1. PL quantum yield of two $MoSe_2$ monolayers deposited onto an indium tin oxide (ITO) coated glass cover slip. The image (a) was taken before inducing a tunneling current through the sample. The image (b) was taken while inducing a tunneling current through the sample and the image (c) was taken several seconds after cutting the tunneling current.

[1] Lien, D.-H. *et al.* Electrical suppression of all nonradiative recombination pathways in monolayer semiconductors. *Science* **364**, 468–471 (2019).
[2] He, Z. *et al.* Quantum plasmonic control of trions in a picocavity with monolayer WS_2. *Science Advances* **5**, eaau8763 (2019).

Electronic Structure Evolution in the Temperature Range of Metal–Insulator Transitions on Sn/Ge(111)

M. N. Nair[1], I. Palacio[2], Y. Ohtsubo[3], A. Taleb-Ibrahimi[4], E.G. Michel[5,6], A. Mascaraque[7], and A.Tejeda[4,8]

[1] Nanoscience Initiative, Advanced Science Research Center, CUNY, New York, USA
[2] Instituto de Ciencia de Materiales de Madrid, CSIC, Madrid, Spain
[3] Grad. School of Frontier Biosciences, Osaka University, Japan
[4] Synchrotron SOLEIL, L'Orme des Merisiers, Saint-Aubin, 91192 Gif sur Yvette, France
[5] Departamento de Física de la Materia Condensada, Univ. Autónoma de Madrid, Spain
[6] Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, Spain
[7] Departamento de Física de Materiales, Universidad Complutense de Madrid, E-28040 Madrid, Spain
[8] CNRS, Université Paris-Saclay, Laboratoire de Physique des Solides, 91405 Orsay, France

*corresponding author: *antonio.tejeda@cnrs.fr*

One-third of monolayer of Sn adatoms on a Ge(111) substrate forms a 2D triangular lattice with one unpaired electron per site. The system presents a metal–insulator transition when decreasing the temperature [1,2] and it is known to exhibit strong electron–phonon coupling at 120–150 K [3]. Herein, a study of the electronic band structure for α-Sn/Ge(111) between 150 and 5 K is reported. Both the experimental Fermi surfaces and the energy dispersions along high symmetry directions as a function of the temperature are presented. At 5 K it is observed a weakly or low-dispersing spectral feature, exhibiting an extended gap in the reciprocal space. This feature is derived from the topmost occupied band, which is metallic at high temperature and which develops a kink associated with the strong electron–phonon coupling. The spectral evolution is partially explained with an increase of the electron–phonon coupling when decreasing the temperature. The increase of the electron–phonon coupling at low temperatures gives light into the new physics of this 2D system. The bandwidth is progressively reduced when reducing the temperature, enhancing the electronic correlation effects, and triggering the Mott transition [4].

[1] R. Cortés, A. Tejeda, J. Lobo, C. Didiot, B. Kierren, D. Malterre, E. G. Michel, A. Mascaraque, Phys. Rev. Lett. 96, 126103 (2006).
[2] R. Cortés, A. Tejeda, J. Lobo-Checa, C. Didiot, B. Kierren, D. Malterre, J. Merino, F. Flores, E. G. Michel, A. Mascaraque, *Phys. Rev. B* **88**, 125113 (2013)
[3] M. N. Nair, I. Palacio, A. Mascaraque, E. G. Michel, A. Taleb-Ibrahimi, A. Tejeda, C. González, A. Martín-Rodero, J. Ortega, F. Flores, *Phys. Rev. B* **107**, 045303 (2023)
[4] M. N. Nair, I. Palacio, Y. Ohtsubo, A. Taleb-Ibrahimi, E.G. Michel, A. Mascaraque, A. Tejeda *Phys. Status Solidi RRL* (2024) https://doi.org/10.1002/pssr.202400041

Functionalization of silicene by small molecules studied by scanning tunneling microscopy

Laurita Florean[1,2], Hervé Cruguel[1], Yves Borensztein[1],
Romain Bernard[1], Fabrice Bournel [2], Geoffroy Prévot[1*]
[1] *Sorbonne Université, CNRS, Institut des NanoSciences de Paris, INSP, 75005 Paris, France*
[2] *Sorbonne Université, CNRS, Laboratoire de Chimie Physique – Matière et Rayonnement, Paris*
*corresponding author: prevot@insp.jussieu.fr

2D-Xenes (where X = Si, Ge, Sn ...), a class of two-dimensional materials of the group IVA, have been the subject of widespread interest owing to their unique electronic properties different from those of the corresponding 3D bulk. Among them, silicene has been particularly studied as Si is one of the basic components of the semi-conductor industry [1]. We have recently synthesized a novel 2D Si allotrope: Dumbbell Silicene (DBSi), which displays a periodic organization of Si adatoms on the silicene surface [2] These adatoms are expected to be preferential adsorption sites for foreign atoms or molecules, that would make possible to tune the electronic properties of the layer.

Using scanning tunneling microscopy (STM), we have studied the functionalization of DBSi with ammonia (NH_3) and triethylamine (TEA) molecules on DBSi grown on Ag(110). Below 200K, NH_3 molecules physisorb on the surface with two atomic configurations: on-top of Si adatoms or between 4 Si adatoms. For higher temperatures, dissociative chemisorption is observed. Our experimental measurements allowed us to determine the difference between energy barriers for desorption or dissociation from the physisorbed state. As concerns chemisorption sites, below 300K, NH_3 molecules are preferentially bounded to Si adatoms (see Figure). Various other configurations are however observed at room temperature. For TEA molecules, a transition between physisorption and chemisorption is also observed, but without a clear preference for chemisorption on adatom sites.

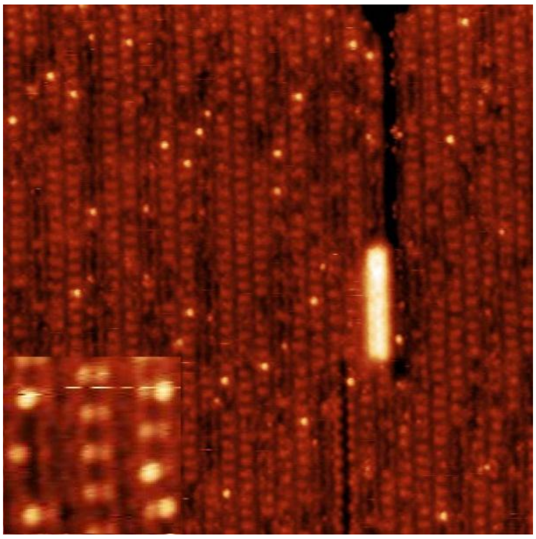

Figure. STM observation of NH_3 adsorption on DBSi at 245K. (50x50 nm^2) for low coverage. White spots correspond to adsorbed molecules. The 5x5 nm^2 inset shows that adsorption mainly occurs on Si adatoms.

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High performance NO_2 gas sensor at room temperature based on a highly compacted ultra-thin WS_2 nanosheets film

Ran Li[1,2], Elmehdi Ould Maina[1,2], Kassioge Dembele[1] and Fatima Z. Bouanis[1,2]
[1] *LPICM, CNRS, Ecole Polytechnique, Institut Polytechnique de Paris, 91128 Palaiseau, France*
[2] *COSYS-IMSE, University Gustave Eiffel, F-77454 Marne-la-Vallée, France*
*corresponding author: ran.li@polytechnique.edu

Transition metal dichalcogenides (TMDs) are a family of semiconducting 2D nanomaterials. Among them, WS_2 stands out due to its theoretically high electron and hole mobilities [1], earning it the reputation of a "beyond graphene and beyond MoS_2" layered material [2]. WS_2 can be easily exfoliated into nanosheets rich in surface active sites, which is crucial for gas sensing performance. In this study, we leveraged this material to develop a next-generation, highly sensitive chemiresistive gas sensor based on WS_2 nanosheets, specifically designed for detecting NO_2 at sub-ppm levels. WS_2 nanosheets were synthesized through a highly efficient and eco-friendly liquid phase shear exfoliation (LPSE)-centrifuge method, with various parameters optimized to achieve a narrow sheet-size distribution. The WS_2 NSs were thoroughly characterized using complementary characterization techniques (UV, DLS, SEM, AFM, TEM, XRD, Raman) to determine their structure and morphology. Spectroscopic and microscopic analyses indicate that the 2D WS_2 NSs were obtained with a low layer number (1-5) and the mean lateral size of 38.7 nm. A self-assembly (SA) method was used to fabricate a highly stacked, continuous WS_2 thin film with a thickness of 20-30 nm. After depositing interdigitated gold electrodes onto the thin film, the assembled device exhibited stable ohmic behavior in both vacuum (500 MΩ) and gaseous environments, demonstrating reliable electrical characteristic. The WS_2-based NO_2 sensor exhibited notable sensitivity (23% at 0.5 ppm) along with reliable reversibility. The response and recovery times of 0.5 ppm NO_2 pulse were measured to be 40 seconds and 1800 seconds, respectively. At room temperature, the sensor's response signal remained stable after four cycles (0.5 ppm NO_2 pulse) and maintained consistent performance for over 40 days, confirming its repeatability and stability. Moreover, the sensor exhibited high selectivity towards NO_2 over other gases. Additionally, the effects of temperature and humidity were studied, confirmed the sensor's stability under real-world conditions. This study highlights the promise of solution-processed 2D thin film for high performance gas sensor applications.

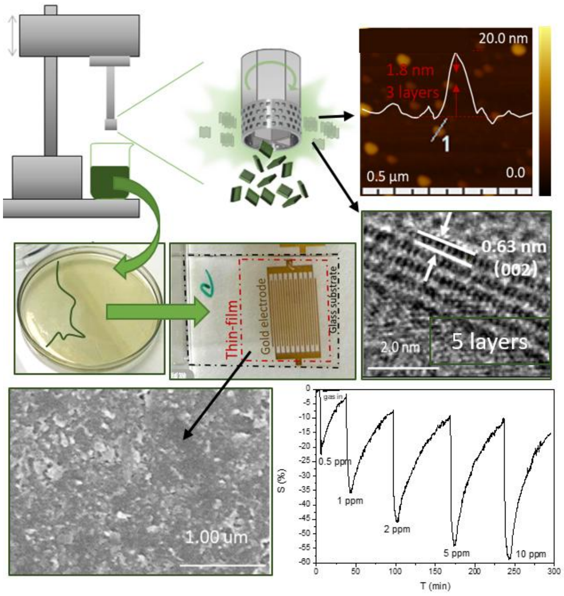

Fig.1. Gas sensor fabrication using LPSE-SA method, WS_2 nanosheets structure, film surface structure and sensing performance.

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[2] Kumar A, Mirzaei A, and Lee M H, Journal of Materials Chemistry A (2024).

Optimization of synthesis and growth of layered ferromagnetic oxides using molten salts method

D. Morley[1,2]*, J.-C. Le Breton[1], P. Turban[1], V. Demange[2]
[1]*Institut de Physique de Rennes – Université de Rennes, CNRS – France*
[2]*Institut des Sciences Chimiques de Rennes – Université de Rennes, CNRS – France*

*corresponding author: dorian.morley@univ-rennes.fr

Spintronics is one of the promisisng ways to further develop electronic systems, more particularly writh the aim to greatly reduce energy consumption while maintaining growing performances. One of the present challenges for the development of 2D-based magnetic tunnel junctions is the synthesis of air stable 2D ferromagnet with Curie point higher than room-temperature.

This presentation focuses on the development of synthesis of 2D-TFCO, doped-titanate oxide nanosheets, an original 2D oxide stable in ambiant atmosphere which could have suitable magnetic properties at room temperature for spintronics uses. TFCO-ONS are produced via the exfoliation of a bulk layered patent oxides of KTFCO, bulk crystals of TFCO obtained by solid state chemistry methods.

Latest results of the optimization of synthesis of KTFCO using molten salts (MS) method will be presented, especially the growth of millimetric single crystals with Curie point above room temperature. Some of the early results of exfoliation of KTFCO crystals as TFCO-nanosheets will also be presented to demonstrate their possible use as nanometrically thin materials suitable in spintronics heterostructures.

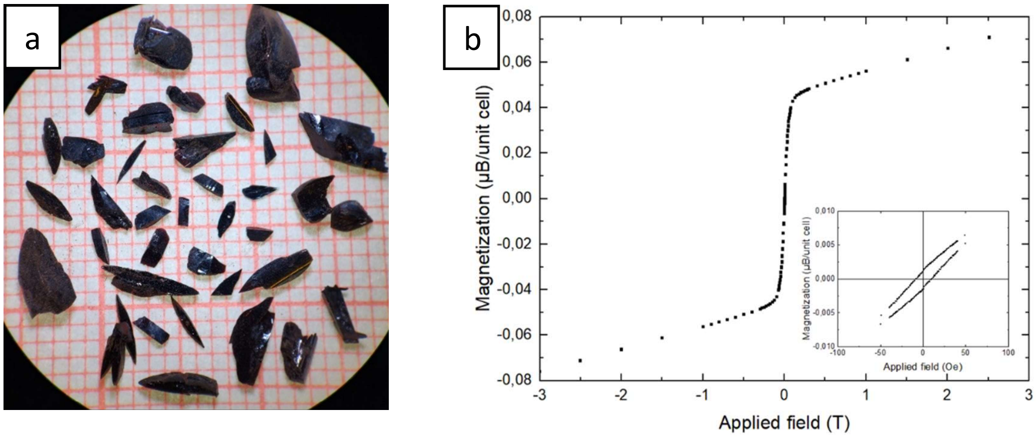

Fig.1. a) Picture of KTFCO bulk crystals grown using molten salts method;
b) Ferromagnetic hysteresis measured at 300K of a bulk crystal of KTFCO (a focus of the hysteresis measured at 300K around the zero-field point is presented as an inset in Fig.1b.).

Phase transition in bilayer WSe2/III-V heterostructure

Meryem Bouaziz[1], Aymen Mahmoudi[1], Niels Chapuis[2], Fabrice Oehler[1], Julien Chaste[1],
François Bertran[3], Iann C. Gerber[4], Gille Patriarche[1], Xavier Wallart[2], Abdelkarim Ouerghi[1]

[1]Université Paris-Saclay, CNRS, Centre de Nanosciences et de Nanotechnologies, 91120, Palaiseau, Paris, France
[2] Univ. Lille, CNRS, Centrale Lille, JUNIA ISEN, Univ. Polytechnique Hauts de France, UMR 8520-IEMN F59000 Lille France
[3]Synchrotron SOLEIL, L'Orme des Merisiers, Départementale 128, 91190 Saint-Aubin, France
[4]Université de Toulouse, INSA-CNRS-UPS, LPCNO, 135 Avenue de Rangueil, 31077 Toulouse, France

*meryem.bouaziz@universite-paris-saclay.fr

Molecular beam epitaxy (MBE) growth of bilayers two-dimensional (2D) materials on conventional 3D semiconductors gives rise to 2D/3D quasi-van der Waals heterostructures. The importance of these heterostructures depends on the properties of the 2D material used. Thus, the stacking and crystalline structure of the bilayer is an important factor that needs investigation. We report a direct observation of a controllable phase transition in bilayer tungsten diselenide (WSe_2) on GaP(111) heterostructure induced by annealing temperature. The crystalline structures of 3R stacking bilayer accompanied by 1T' phase and the 2H phase were characterized using reflection high energy electron diffraction (RHEED). The phase transition mechanism is confirmed using the electronic properties by XPS and ARPES. This temperature-induced crystalline phase transition makes the WSe_2 bilayer an ideal platform for controlling topological phase transitions in 2D materials[1-3].

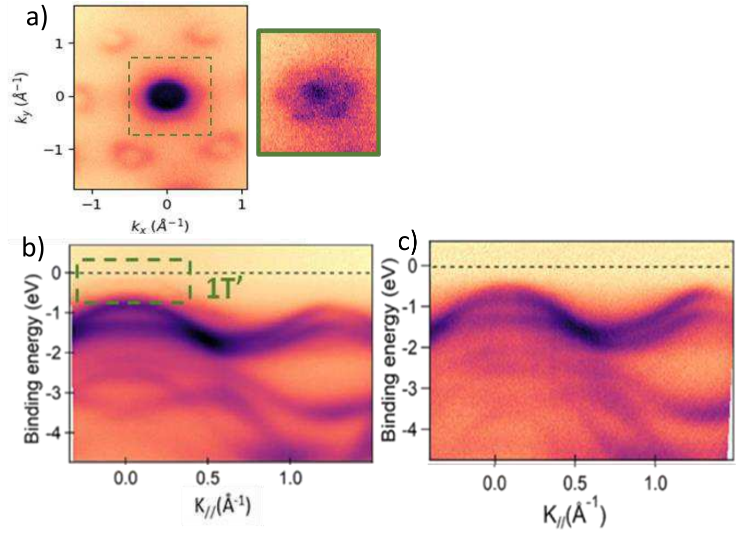

Figure 1: a) Fermi surface of the WSe_2 bilayer showing the Γ point surrounded by the 6 K points. A moiré system can be distinguished in the low-scale image, confirming the 1T' phase. Comparison of the band structure of WSe_2 at low temperature (b)before and(c) after annealing at 600°C, illustrating the transition from metallic 1T'phase to hexagonal 2H phase.

[1] Aymen Mahmoudi, Meryem Bouaziz, Niels Chapuis, Geoffroy Kremer, Julien Chaste, Davide Romanin, Marco Pala, François Bertran, Patrick Le Fèvre, Iann C. Gerber, Gilles Patriarche, Fabrice Oehler, Xavier Wallart, Abdelkarim Ouerghi, ACS Nano 17, 21307 (2023).

[2] Aymen Mahmoudi, Meryem Bouaziz, Anis Chiot, Gaia Di Berardino, Nathan Ullberg, Geoffroy Kremer, Pavel Dudin, José Avila, Mathieu Silly, Vincent Derycke, Marco Pala, Iann C. Gerber, Julien Chaste, Fabrice Oehler and Abdelkarim Ouerghi, PHYSICAL REVIEW B 108, 045417 (2023).

[3] “Temperature induced phase transition in bilayer WSe_2/GaP heterostructure”. Meryem Bouaziz, Aymen Mahmoudi, Niels Chapuis, Fabrice Oehler, Julien Chaste, François Bertran, Iann C.Gerber, Gilles Patriarche, Xavier Wallart, Abdelkarim Ouerghi ; in progress

Renforcement de l'adhésion moléculaire pour l'assemblage de verres de silice : rôle de l'activation des surfaces par plasma

V. Ménard[1], J. Debray[2], C. Hecquet[3], F. Fournel[4], A. Talneau[5], A. Maurel-Pantel[6], F Lebon[6]
[1] *Laboratoire CIMAP, 6 Boulevard Maréchal Juin 14050 Caen France*
[2] *Institut Neel, CNRS | UGA 25 avenue des Martyrs - 38042 - Grenoble – France*
[3] *Laboratoire Charles Fabry (LCF UMR8501), CNRS, Palaiseau, France*
[4] *CEA LETI, CEA, Grenoble, France*
[5] *CNRS - Centre de Nanosciences et de Nanotechnologies (Palaiseau, France*
[6] *Aix Marseille Université, CNRS, Centrale Marseille, LMA, Marseille, France*
*corresponding author: vivien.menard@ensicaen.fr

La préparation des surfaces avant mise en contact pour réaliser un assemblage peut être optimisée de façon à augmenter leur adhérence à basse température de recuit de collage. Pour des surfaces planes, non rugueuses, et propres de toute particule ou contamination chimique, le plasma contribue à leur activation.

Cette méthode est très utilisée pour la préparation des surfaces de matériaux semi-conducteurs [1-3]. On utilise des plasmas Ar, O_2 ou N_2. La préparation de surfaces de verre par plasma avant assemblage a été reportée [4-5], sans toutefois détailler les mécanismes mis en œuvre pour renforcer l'adhésion.

L'étude poursuivie ici cherche à identifier les mécanismes mis en jeu lors de l'assemblage de surface traitées par plasma, puis une fois les assemblages obtenus, mesurer leur tenue mécanique en traction/cisaillement de façon à estimer l'énergie du joint d'interface.

Des mesures XPS -X Ray Photoelectron Spectroscopy- des surfaces traitées par plasma ont permis d'identifier les liaisons de surface qui pourraient intervenir dans le renforcement de l'adhésion.

Fig.1. Assemblages de verre de silice dont les surfaces ont été traitées par plasma (*J. Debray, Institut Néel, Grenoble*)

On voit ci-contre 3 assemblages de verres de diamètre 50mm, épaisseur 22mm.
L'interface n'est pas visible, il ne présente aucune teinte car les 2 surfaces sont parfaitement associées.

Les mesures mécaniques de la tenue de ces assemblages sont en cours.

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Self-Trapped Excitons in 2D Hybrid Perovskites

F. Johora[1], M. Roux[1], G. Trippé-Allard[2], E. Deleporte[2], O. Plantevin[1]
[1]*Laboratoire de Physique des Solides UMR8502, Orsay, France*
[2]*LUMIN, UMR9024, Orsay France*
*corresponding author: Olivier.plantevin@universite-paris-saclay.fr

Two-dimensional (2D) organic-inorganic lead halide perovskites have gained significant interest for optoelectronic applications [1]. By studying the temperature dependence of their optical spectra, we gained insights into their excitonic properties. Photoluminescence (PL) measurements of $(PEA)_2(CH_3NH_3)_{n-1}[Pb_nI_{3n+1}]$ $(PEA=C_6H_5(CH_2)_2NH_3)$ (simply PEPI) single crystals revealed both narrow and broad emissions. Analysis of the narrow band to band emission and its temperature dependence indicates an exciton binding energy ∼180 meV, which is 10 times higher than in 3D MAPbI3, indicating the strong excitonic character. As shown in Fig.1, the broad emission signature emerges upon cooling below 260 K. The non-monotonic behaviour of the peak PL position satisfies the Bose-Einstein equation. Analysis of the broad emission line demonstrates a strong exciton-acoustic phonon interaction. This emission can be associated to self-trapped excitons where the excitons get trapped in long-lived states (up to 4.5 ms at 10 K) due to lattice deformation. By comparing single crystals to grinded powder, we conclude that the STE is not enhanced by the presence of defects and rather rely on an intrinsic mechanism as was recently debated [2].

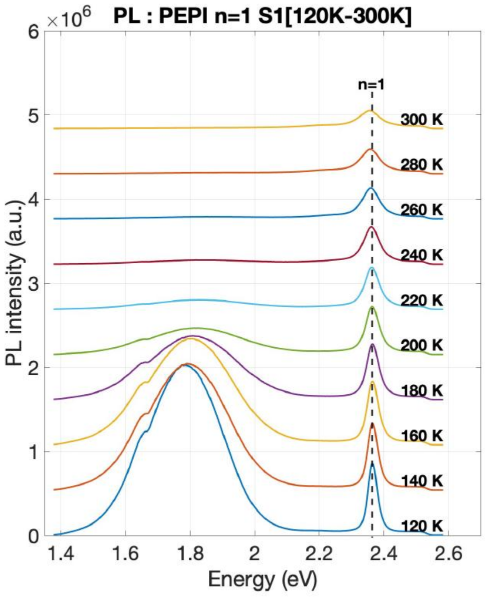

Fig.1. Temperature dependence of the PL emission from PEPI single crystal in the range 300 K-120 K under laser excitation at 448 nm.

[1] L. Mao, C.C. Stoumpos, M. Kanatzidis, J. Am. Chem. Soc. (2019) 141, 1171-1190.
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Core-level binding energy shifts in ultrathin alkali-halide films on metals

S. Le Moal[1], I. Krieger[2], R. Kremring[2], S. Weiß[3,4], X. Yang[3,4], S. Soubatch[3,4], F. S. Tautz[3,4,5], M. Silly[6], A. G. Borisov[1], M. Sokolowski[2], and E. Le Moal[1]
[1]*Université Paris-Saclay, CNRS, Institut des Sciences Moléculaires d'Orsay, Orsay, France*
[2]*Institut für Physikalische und Theoretische Chemie der Universität Bonn, Bonn, Germany*
[3]*Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, Jülich, Germany*
[4]*Jülich Aachen Research Alliance (JARA)-Fundamentals of Future Information Technology, Jülich, Germany*
[5]*Experimental Physics IV A, RWTH Aachen University, Aachen, Germany*
[6]*Synchrotron-SOLEIL, Saint-Aubin, Gif sur Yvette, France*
*corresponding author: eric.le-moal@universite-paris-saclay.fr

We present an experimental and theoretical analysis of the core-level binding energy shifts in metal-supported ultrathin KCl films, i.e., a case from a broader class of few atom-thick, wide-bandgap insulating layers that is increasingly used in nanosciences and nanotechnologies. Using synchrotron-based high-resolution photoemission spectroscopy (HRPES) measurements, we identify the different contributions to the core-level binding energy shifts for the Cl– anions and K+ cations of two to three atomic layer-thick KCl films grown on Ag(100). The distances of the Cl– and K+ ions of the first two atomic layers of the KCl film from the metal substrate are determined from normal incidence X-ray standing wave measurements. We also calculate the core-level binding energy shifts using an analytical electrostatic model and find that the theoretical results are in agreement with the experimental HRPES results only when polarization and substrate induced image charge effects are taken into account. Finally, our results evidence the effect of the third atomic layer of the KCl film, which partially covers and screens the first two atomic layers of KCl wetting the metal substrate..

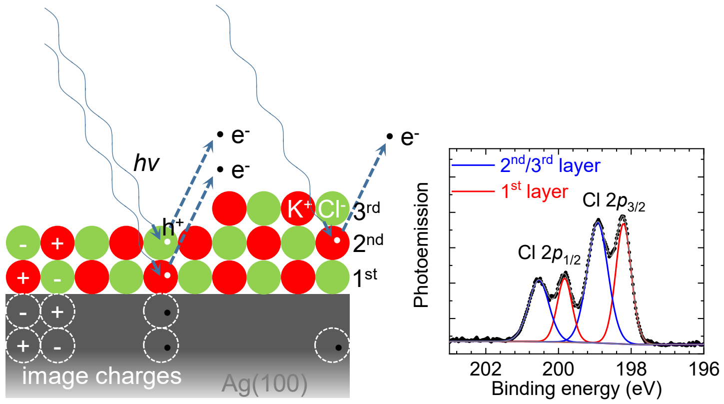

Fig.1. Schematic of the photoemission experiment. HRPES spectra showing the shifted contributions from the Cl 2p core levels of the atoms in the first and second/third atomic layers of the KCl thin film.

[1] Séverine Le Moal, Ina Krieger, Roman Kremring, Simon Weiß, Xiaosheng Yang, Serguei Soubatch, F. Stefan Tautz, Mathieu Silly, Andrei G. Borisov, Moritz Sokolowski, and Eric Le Moal, J. Phys. Chem. C **127**, 50, 24253–24265 (2023).

Engineering surface band bending in rutile TiO_2 through defect manipulation

A. Levy[1], R. Lazzari, Greg Cabailh[1], J. Jupille[1] and S. Guilet[1]
[1]*Institut des Nanosciences de Paris, Sorbonne Université, CNRS, Paris, France*
*corresponding author: gregory.cabailh@sorbonne-universite.fr

Surface band bending (SBB) is a critical parameter influencing charge separation and transport in photocatalytic applications of semiconductors like TiO_2. Our study investigates the contributions of surface oxygen vacancies (O_{vac}) and subsurface titanium interstitials (Ti_{int}) to SBB in rutile $TiO_2(110)$, aiming to control and optimize its magnitude. Previous experiments at DIAMOND's I09 beamline demonstrated our ability to control SBB by inducing Ti_{int} segregation via soft-annealing, with results closely aligning with theoretical estimates [1-3] (up to -0.4 eV across ~8 nm). We observed distinct SBB profiles modulated by Ti_{int} segregation and subsequent O_2 exposure, suggesting that precise manipulation of defect densities can effectively tune SBB [3–5].

Hard X-ray photoelectron spectroscopy (HAXPES) was used to investigate the SBB profile under varied defect conditions. SBB profiles of both sputtered and chemically prepared TiO_2 surfaces are compared, examining the stability of engineered SBB closer to environmental conditions. This comprehensive study aims to establish a robust methodology for SBB manipulation in TiO_2, offering insights into stable photocatalytic interfaces [6,7].

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Etude de la répartition du poids spectral en ARPES avec le logiciel chinook

C.L. NDJIMI[1], G. KREMER[1], B. KIERREN[1], Y. FAGOT REVURAT[1] et D. MALTERRE[1]
[1]*Institut Jean Lamour, Université de Lorraine, Nancy, France*
*corresponding author: Cynthia.ndjimi@univ-lorraine.fr

Les propriétés physiques (transport, magnétiques etc.) des solides cristallins dépendent des excitations électroniques qui peuvent être obtenues expérimentalement par plusieurs méthodes spectroscopiques en particulier la photoémission résolue en angle (ARPES) [1,2]. Dans l'approximation des électrons indépendants, la structure de bande (i.e. les relations de dispersions $E\ (\vec{k})$) peut être obtenue par l'approche de la fonctionnelle de la densité (DFT) [3]. Les calculs DFT sont souvent directement comparés aux mesures ARPES. Cependant, le poids spectral de l'ARPES n'est pas périodique dans l'espace réciproque [4], ce qui complique la comparaison directe entre les spectres ARPES et les structures de bandes calculées. En effet, cette non-périodicité du poids spectral est due aux éléments de matrices à un électron provenant de l'Hamiltonien d'interaction électron- photons. Le poids spectral dépend de la polarisation, de l'énergie des photons et de la géométrie de l'expérience. Ainsi, En 2019, Ryan P. Day a développé le logiciel **chinook** [5] capable de simuler les cartes d'intensités de spectres ARPES sur un matériau dont la structure de bande est modélisée en liaisons fortes. Dans ce poster nous, présenterons l'effet des éléments de matrice sur la répartition du poids spectral en ARPES en utilisant ce logiciel chinook. Nous commencerons tout d'abord par présenter les résultats de simulation des cartes d'intensité ARPES obtenus avec un modèle académique de réseau carré à deux atomes par maille en explicitant l'influence de la polarisation des photons et de la géométrie de l'expérience sur la répartition du poids spectral [6]. Nous terminerons par une comparaison entre les simulations de cartes d'intensité ARPES et les spectres d'ARPES expérimentaux sur plusieurs matériaux bidimensionnels.

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In situ photoemission spectroscopies to reveal surface transfer doping on hydrogenated milled nanodiamonds

C. Njel[1,2], H. A. Girard[2], M. Frégnaux[1], D. Aureau[1], J.-C. Arnault[2],
[1] *Institut Lavoisier de Versailles (ILV), UMR 8180, CNRS, UVSQ - Université Paris-Saclay, 78000, Versailles, France*
[2] *Université Paris-Saclay, CEA, CNRS, NIMBE, 91191, Gif sur Yvette, France*
*corresponding author: jean-charles.arnault@cea.fr

Nanodiamonds (ND) exhibit exceptional chemical, electronic, thermal, and optical properties, making them valuable for applications in nanomedicine, energy, quantum technologies, advanced lubricants, and polymer composites. ND inherits semiconducting properties from bulk diamond. The surface chemistry strongly influences their electronic properties leading to a large energy shift in their band structure (valence and conduction bands) and turning the electronic affinity from positive to negative for oxidized and hydrogenated diamonds, respectively [1]. Surface analysis techniques such as X-ray photoemission spectroscopy (XPS), ultraviolet photoemission spectroscopy (UPS) and reflection electron energy loss spectroscopy (REELS) are critical for understanding the surface properties of nanomaterials, including nanodiamonds [2].

This study investigates hydrogenated milled nanodiamonds (H-MND) by integrating UPS and XPS measurements with REELS. Through *in situ* annealing within an ultra-high vacuum (UHV) chamber, we examine the impact of surface termination on surface conductivity, focusing on the role of adsorbates. Our findings reveal that a surface transfer doping mechanism, akin to that observed in bulk diamond, governs a pseudo p-type conductivity in H-MND. The conductivity dependence on ambient exposure, water, and subsequent annealing demonstrates its reversibility (Figure 1). The study also discusses the nature of electron acceptors and the influence of ND facets on conductivity [3].

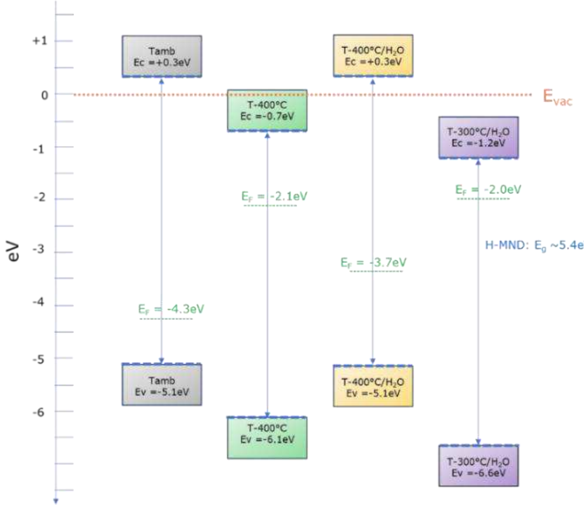

Fig.1. Band diagrams of H-MND extracted from the UPS spectra before annealing (Tamb), after UHV annealing at 400 ˚C (T-400 ˚C), after UHV annealing at 400 ˚C and dropcasted of H_2O (T-400 ◦C/H_2O), and after UHV annealing at 300 ˚C (H_2O/T-300 ˚C).

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