JSI-2026

Résumés des posters

Le numéro avant le titre indique le panneau sur lequel le poster sera affiché

1. Structure of $Co_xCu_{1-x}O(001)$ thin films grown on $SrTiO_3(001)$ by oxygen plasma assisted molecular beam epitaxy

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Ultrathin films of a tetragonal (t) CuO phase were grown several years ago in epitaxy on $SrTiO_3(001)$ by pulsed laser deposition[1]. This new phase is regarded as an archetypal model to explore the ground state physics of Mott insulators and as a promising platform to understand the mechanisms of high-T_C superconductivity in cuprates. t-CuO is also predicted to have a high Néel temperature, in contrast with the CuO monoclinic phase, thanks to an increased super-exchange interaction, related to its structure. Doping t-CuO with magnetic elements should result in a magnetic semiconductor at room temperature.

The elaboration of CuO films in vacuum conditions requires an activated form of oxygen. We grew t-CuO(001) and t-$Co_xCu_{1-x}O(001)$ films by oxygen plasma assisted molecular beam epitaxy. We demonstrated that this phase is stable for film thicknesses above 6 nm, and we solved its structure by *in situ* x-ray diffraction, showing that it is in coherent epitaxy on the $SrTiO_3(001)$ substrate. We determined exactly the tetragonal distortion c/a= 1.342(2). This ratio value is crucial for the 2D character of its electronic structure and reinforces the similarity with high-T_C cuprates. We also showed, using resonant x-ray diffraction, that Co replaces Cu in the film structure, at least up of 10% of substitution. Magnetic characterization is in progress.

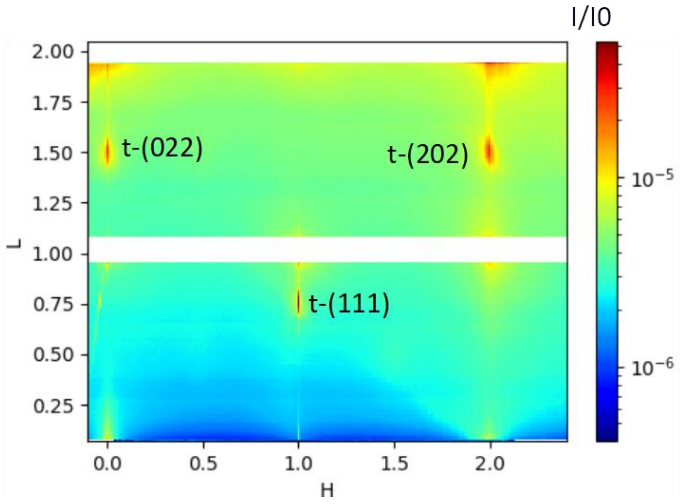

Fig.1. XRD intensity map of a $Co_{0.1}Cu_{0.9}O/SrTiO_3(001)$ film projected in the *HL* plane. The tetragonal phase (022), (111), and (202) peaks are indicated

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2. Charge density waves in metallic/insulating phases of monolayer $TaSe_2$/GaP

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Transition Metal Dichalcogenides (TMDs) are a great family of materials that exhibits a wealth of electronic properties. For instance, TMDs can be metallic as well as insulator or superconductor. They are also prone to exhibit charge density waves (CDW). Among the TMDs, 1T-$TaSe_2$ displays a star-of-David $\sqrt{13} \times \sqrt{13}$ charge density wave which induces an unusual strong correlation effect: an insulating surface layer while the bulk remains metallic [1]. Some studies point out the emergence of a Mott insulating phase for a 1T-$TaSe_2$ monolayer [2,3]. This Mott insulating phase persists in few layers system and disappears in the bulk of thick samples. By contrast, the 1H-$TaSe_2$ remains metallic, in agreement with DFT calculations, and becomes superconducting at low temperature.

In 2016, Ma et al. [4] showed that STM voltage pulses could locally drive a transition from an insulating state with the famous star-of-David CDW to a metallic state with a mosaic charge density wave. These measurements were performed on bulk materials for which only the surface is insulating while the bulk is metallic. This intriguing pulse induced insulator to metal transition could be useful for drawing electronic circuits on single atomic layer, of few atomic layers, TMDs.

In this frame, we have performed scanning tunneling microscopy/spectroscopy experiments to investigate electronic properties of monolayers of $TaSe_2$ grown by Molecular Beam Epitaxy (MBE) on a GaP(111) surface. We are exploring samples consisting in mixed phases of 1T and 1H-$TaSe_2$ domains covering approximately one monolayer, with few bilayers areas. Above the 1T-$TaSe_2$ flakes, voltage pulses can be done in order to try to induce phase transitions from insulating to metallic state.

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[2] H. Koussir et al., Large-Area Epitaxial Mott Insulating 1T-$TaSe_2$ Monolayer on GaP(111)B, Nano Lett. **23**, 9413 (2023).

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[4] L. Ma et al., A metallic mosaic phase and the origin of Mott-insulating state in 1T-TaS2, Nat Commun **7**, 10956 (2016).

3. Insights into Clean and Hydrated Low-Index $Rb_2Ti_2O_5$ Surfaces

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The layered oxide $Rb_2Ti_2O_5$ [1,2] has recently emerged as a promising solid electrolyte, displaying exceptional ionic conductivity and dielectric response at room temperature under humid conditions [3,4]. Although these macroscopic properties are known to depend on water content [5], the atomic-scale behavior of its surfaces—key to understanding interfacial reactivity and ion transport—remains largely unexplored. Using density functional theory (DFT), we examine the atomic structure, thermodynamic stability, and hydration reactivity of the three low-index surfaces, (100), (010), and (001), of $Rb_2Ti_2O_5$ [6], focusing on stoichiometric, unreconstructed terminations. Among them, the (001) surface is found to be the most stable, with a surface energy significantly lower than that of conventional oxides. Only minimal structural and electronic rearrangements occur upon cleavage, consistent with the material's quasi-two-dimensional character. Water adsorbs spontaneously in molecular form, assembling into ordered layers held by short hydrogen bonds (Fig.1), with minor perturbation of the surface. Under increased hydration, the (001) termination reaches a near-zero surface energy, indicating spontaneous exfoliation into hydrated sheets. The pronounced outward displacement of Rb atoms upon hydration could facilitate alkali-cation solvation, in line with experimental observations [7]. This trend is further supported by recent evidence for a favorable substitution mechanism of Rb by H atoms. Hydration can also strongly modify the Ti environment at the (001) surface, allowing its coordination to increase from five to six following water dissociation. Overall, hydration reduces surface stress and stabilizes terminations, yielding thermodynamically accessible states even at low water partial pressures. The (100) surface is highly reactive, forming spontaneously hydroxylated termination with water adsorption. The hydrated (010) surface hosts several metastable configurations and can undergo hydroxylation through low-barrier water dissociation. These results underscore the dual role of water: stabilizing surfaces while simultaneously enabling proton incorporation and the formation of additional chemical species within the material. This work lays the groundwork for future studies of hydration-driven processes, surface dynamics, ion transport, and machine-learned simulations. We would be delighted to present this work at your conference, as it could stimulate meaningful discussions on ionic conductors and surface reactivity in emerging energy materials.

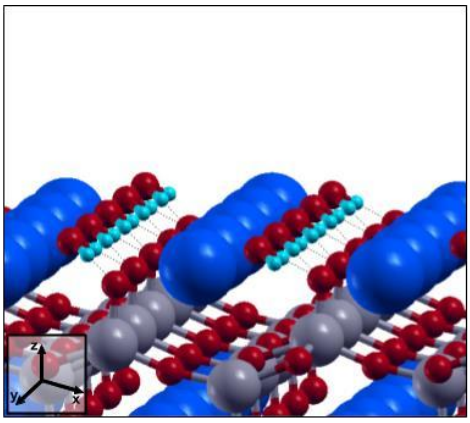

Fig.1. Hydrated (001) surface configuration represented using XCrysDen [8].

[1] S. Andersson and A.D. Wadsley,Nature, 192:551–552 (1961)
[2] R. Federicci *et al.*, Acta Cryst. B, 73(6):1142 (2017)
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[8] Anton Kokalj. Journal of Molecular Graphics and Modelling, Volume 17(Issues 3–4), 1999.

4. High-Tc Ferromagnetic Oxide Nanosheets for Spintronic Applications

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Spintronics intends to further develop electronic systems with the aim of reducing energy consumption while maintaining growing performances. In this framework, 2D oxide materials are a promising platform offering model properties ranging from high-k 2D dielectrics [1] to 2D ferroelectrics [2] or 2D ferromagnets [3] while being intrinsically air stable, an overall key asset for 2D spintronics.

This presentation focuses on the development of 2D-TFCO ($[Ti_{0.8-x/4}Fe_{x/2}Co_{0.2-x/2}O_2]^{0.4-}$) doped-titanate oxide nanosheets, an original 2D oxide stable in ambient atmosphere with ferromagnetic properties at room temperature [3]. TFCO oxide nanosheets are produced via the exfoliation of the bulk layered parent oxide KTFCO ($K_{0.4}Ti_{0.8-x/4}Fe_{x/2}Co_{0.2-x/2}O_2$), synthesized by solid-state chemistry methods. The optimization of synthesis parameters has led to the growth of millimetric KTFCO single crystals (see Fig.1a) suitable for bulk properties analysis prior to the exfoliation of large area TFCO nanosheets.

Latest results on KTFCO crystals characterizations will be presented, especially their magnetic properties with Curie point above room temperature. Structural properties of the layered phase will also be presented. Exfoliation of KTFCO crystals into TFCO-nanosheets (Fig.1b) will be demonstrated as a first step towards the integration of this 2D ferromagnetic insulator as a functional material in spintronics heterostructures (Fig.1c). Finally, a specific focus will be dedicated to the investigation of the electronic, magnetic, transport and magneto-transport properties of 2D-TFCO single and multilayers.

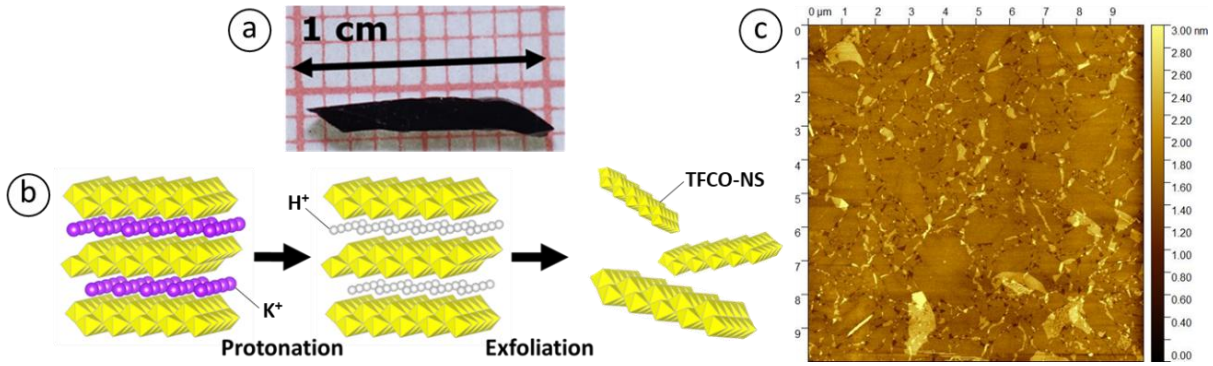

Fig.1. a) Picture of millimetric KTFCO layered crystal grown using molten salts method;
b) Detailed diagram of KTFCO chemical exfoliation process; c) AFM image of single-layer film of TFCO nanosheets

[1] M. Osada, T. Sasaki. Adv. Mater. **2**, 210-228 (2012).

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5. Electrophoretic deposition of octahedral molybdenum clusters and graphene oxide layers for antibacterial photoinactivation

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In the current context of microbial resistance to commonly used treatments, it is imperative to find alternatives to combat infections. A promising approach is to use antimicrobial coatings containing molecules capable of inactivating the proliferation of microorganisms through the application of visible light (photodynamic inactivation or PDI). This thesis' works, supported by the Rennes University, are performed under the frame of the EIG Concert Japan PHOTOMOS-H2O with our partners: IIC in the Czech Republic, the Waseda University in Japan, the University of Orleans and CNRS in France. The main aim of this work is to design and study innovative hybrid coating films capable of efficiently inhibiting bacterial growth. To achieve this, we primarily focus on the integration of light-induced singlet oxygen generators [Fig. 1]: octahedral molybdenum cluster complexes with the formula $[Mo_6I_8X_6]^{2-}$ (Mo_6) on graphene oxide (GO) [1-3]. To obtain thin layers integrating these two elements, several implementation techniques are being explored. Electrochemical deposition (ECD), electrophoretic deposition (EPD) and dip-coating techniques are promising for obtaining antibacterial coatings effective against a wide range of bacteria (Gram-negative and Gram-positive) and biofilms. The hybrid films are characterised by various techniques such as XRD, SEM, EDS, XPS, Raman spectroscopy, and, most importantly, photoluminescence measurements showing whether nanocomposites are capable of producing reactive oxygen species (ROS), as singlet oxygen O_2 ($^1\Delta_g$), responsible for the inhibition of bacterial growth. This study highlights the potential of hybrid coatings based on Mo_6 and GO to combat bacterial infections, offering a promising alternative in the face of increasing antibiotic resistance.

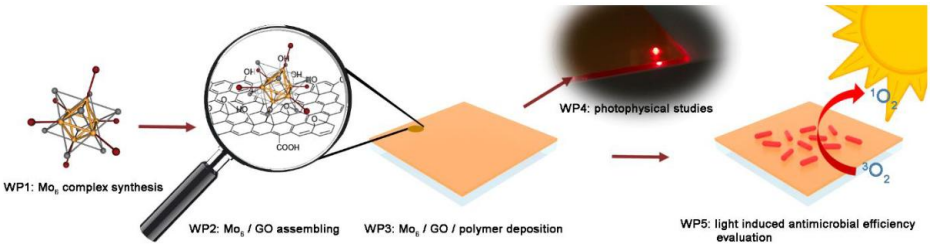

Fig.1. Principle of the hybrid system

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[2] S. Khlifi, J. Bigeon, M. Amela-Cortes, N. Dumait, H. Akdas-Kilic, G. Taupier, S. Freslon, S. Cordier, S. Derien, M. Achard, G. Loas, Y. Molard, J. Mater. Chem. C. **9 (22)**, 7094 (2021).
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6. First-Principles Insights into Band Gaps, Surface Stability, and Energy Levels in Halide Perovskites

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Halide perovskite materials have attracted considerable attention as efficient absorbers for solar cells, light-emitting diodes, and photodetectors, owing to their tunable band gaps, large absorption cross sections, and long carrier lifetimes and diffusion lengths [1]. Precise control of band gaps and energy-level alignment is therefore crucial for optimizing and device performance and efficiency. In this context, accurate predictive simulations play a key role in exploring and tailoring material properties.

In this presentation, we provide a theoretical perspective based on ab initio density functional theory (DFT) simulations on the performance of the doubly screened dielectric-dependent hybrid (DSH) functional for band-gap predictions in halide perovskites [2]. We demonstrate that the DSH functional, which employs material-dependent mixing parameters derived from macroscopic dielectric constants [3], yields accurate band-gap predictions for three-dimensional halide perovskites only when local structural disorder is properly accounted for [4]. For quasi-2D layered perovskites, dielectric screening must be tailored to the band alignment to obtain reliable band gaps. We further show that the HSE functional significantly underestimates band gaps, exhibiting a larger mean absolute error than PBE0 for both 3D and quasi-2D halide perovskites. This discrepancy is attributed to the lack of non-local long-range screening in HSE, which is essential for accurately modeling halide perovskite materials.

Finally, we investigate the non-polar (001) surfaces of vacancy-ordered double perovskites [5,6], focusing on the impact of different surface terminations on surface stability and surface states. The absolute energy levels of the most stable surfaces are computed at the DSH level and compared with available experimental data. This analysis enables the identification of promising charge-transport layer candidates for prototypical perovskite absorbers in photovoltaic and light-emitting device applications.

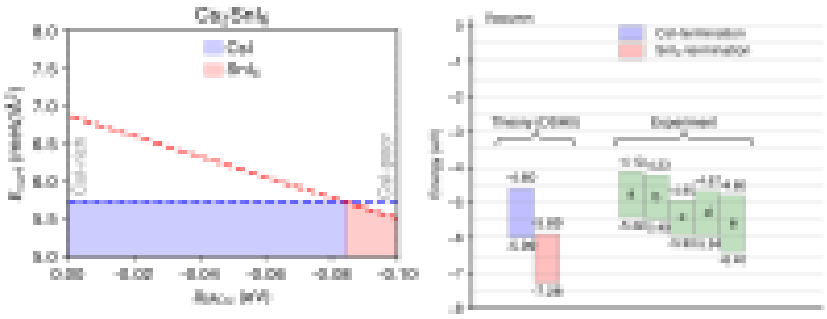

Figure: (left) Surface stability of Cs_2SnI_6 with two terminations, and (right) energy level alignment of the two terminations from theory and experiments.

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7. Development of epitaxial growth of WTe_2 for spin-orbitronics applications

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2D Transition metal dichalcogenides (TMDs) have created huge research interest due to their unique properties and potential for various applications in energy, electronics, photonics, and spintronics. TMDs are mainly obtained through mechanical or chemical exfoliation of bulk crystals into thin atomic layers. Despite challenging, epitaxial growth of these materials offers significant advantages, including the production of highquality films, possible long range in-plane ordering and precise control over layer thicknesses, making it more suitable for applications [1]. Insulating substrates like sapphire (Al_2O_3) are important for several reasons: electrical insulation, reduced (if any) charge transfer, optical transparency, size, crystalline symmetry (a-plane, c-plane, r-plane and m-plane) [2]. TMDs share MX_2 structure (M=W, Mo and X=Te, Se, S). Among TMDs, WTe_2 is the only one for which the Td phase is the most energetically favored [3]. It has been predicted to be a quantum spin Hall insulator in the monolayer regime with bandgap opening due to spin-orbit coupling [4] and ferroelectric down to 2 ML [5]. On the other hand, bulk WTe_2 has been predicted and still arguably evidenced to show type-II Weyl semimetal properties [6]. This calls for a precise investigation of thickness-dependent electronic properties and the development of the growth on insulating substrates of this highly promising material for all-electrically controlled spin-orbitronics applications.

In this study, we elaborate WTe_2 films on sapphire (a-plane (11-20)) by molecular beam epitaxy (MBE). X-ray diffraction (XRD), x-ray reflectivity (XRR) and Raman spectroscopy have been performed to characterize the growth properties of WTe2 films. Results obtained by W and Te co-deposition first showed films of polycrystalline nature due to either a Te deficit or an excess of W in the composition. High temperature annealing (≈600°C) under Te environment is necessary to improve the growth, which allowed us to obtain more crystalline films (fig a). XRD shows a peak at about 12.52° in 2Θ corresponding to the (002) WTe_2 plane family (fig b), XRR allows us to measure the thickness of the layer (fig c) and Raman spectroscopy shows well defined peaks of WTe2 in good agreement with previous works performed on exfoliated samples [7]. Preliminary results of WTe_2 films obtained by post- growth tellurization of W layers will be presented. We have also elaborated several samples (different thicknesses) of WTe2/ML-Graphene/SiC by MBE [8] for AngleResolved Photoemission Electron Spectroscopy (ARPES) and X-ray Photoelectron Spectroscopy (XPS) measurments. (ARPES) shows electron-pockets (for 1-ML and 4-ML) at the Fermi level, in agreement with DFT calculations performed on free-standing Td-WTe2 and previous reports [9]. This confirms the crystalline quality of the films.

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Et al. Nat Commun 5, 4214 (2014) [4] Qian, X. et al. Science 346, 1344–1347 (2014).
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8. Deposition and characterizations of lead-free ferroelectric and antiferroelectric oxide thin films for electric field driven ultrafast phase-change materials

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Artificial intelligence (AI) is a booming field, and research is intensifying to develop tools more and more efficient and less energy-intensive. Neuromorphic computing, inspired by the working of the human brain, could revolutionize AI capabilities while significantly reducing its energy consumption. However, this requires materials with ultrashort response times, in the order of picoseconds, as well as multiple stable states. These properties can be found in particular in phase-change materials (PCM). In this project, we are studying in particular two lead-free ferroelectric and antiferroelectric PCM, KTN ($KNbO_3$-$KTaO_3$) and AKN ($AgNbO_3KNbO_3$), chosen for the richness of their phase diagram and their potential for many applications [1]. One of the main objectives is to produce crystalline quality thin films and to study their phase transitions.
To achieve this, thin films of KTN, of different compositions were synthesized by Pulsed Laser Deposition in order to target different Curie temperatures (figure 1). Structural characterizations such as X-ray diffraction and scanning electron microscopy coupled with energy dispersive X-ray spectroscopy were first carried out to determine the composition and crystallized phases of the thin films. Special attention is paid on the crystallographic orientation of the films as well as the substrate-film structural relationships, possibly epitaxial like. Local investigations by high-resolution studies using (scanning) transmission electron microscopy with electron energy-loss spectroscopy will complete the structural elemental and electronic studies of the different films. Finally, optical characterizations, in particular by terahertz spectroscopy, and electrical characterizations, will be performed in order to deeply investigate the material, the transitions and the interaction with the THz beam in view of further investigation in ultrafast regime.

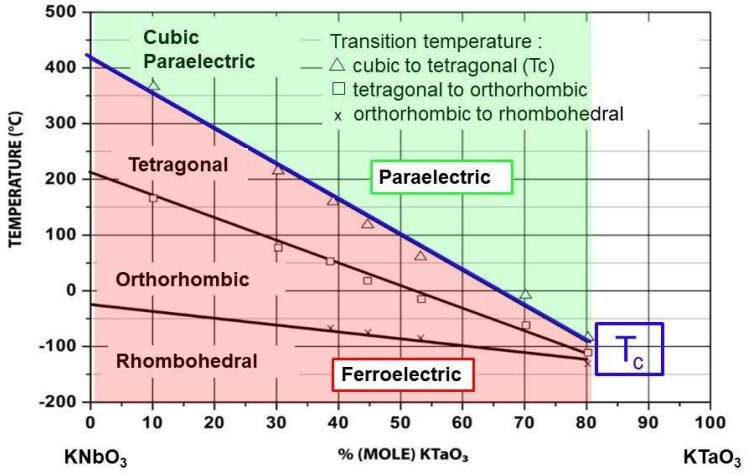

Figure 1: $KNbO_3$-$KTaO_3$ (KTN) phase diagram adapted from ref [1]. The blue line indicates the PE-to-FE phase transition.

Authors acknowledge the French National Research Agency for the financial support in the project FastPHASE No. ANR-24-CE30-2899.

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9. Real-time monitoring of thin film growth by GIFAD: a gentle probe of growth mode, structural properties and phase transitions

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Designing and developing thin-film heterostructures with controlled properties are major challenges for nanoscience and nanotechnology. The development of efficient and discriminating fabrication processes requires sensitive tools capable of providing refined information on the properties of the layer in real time during growth. RHEED (Reflection High Energy Electron Diffraction) contributed significantly to the rise of MBE (Molecular Beam Epitaxy) in the 1980s and 1990s. Despite its many advantages, RHEED reaches its limits with fragile materials and ultra-thin layers, in addition to the complexity related to the dynamical character of the electron-surface interaction.
As an alternative and complement, GIFAD (Grazing Incidence Fast Atom Diffraction), probes primarily valence electrons and is therefore extremely sensitive to subtle variations in the electron density distribution within the lattice. This feature allows clear identification of phase transitions without any change of the lattice parameter. Beyond its effectiveness in characterizing inorganic semiconductors, both in static [1] and dynamic mode [2], it has also been shown effective for monitoring the growth of organic layers without any damage [3].
As good illustrations of the capabilities of GIFAD, we will show results from heterostructures of 2D materials (PbI_2/Graphene, see figure 1) and hybrid halide perovskites ($MAPbI_3$) and its component materials (PbI_2 and CH_3NH_3I). In particular, the growth of $MAPbI_3$ layers in UHV represents a difficult challenge [4]; our results shed a new light on the crystallization dynamics of these fragile and complex systems.

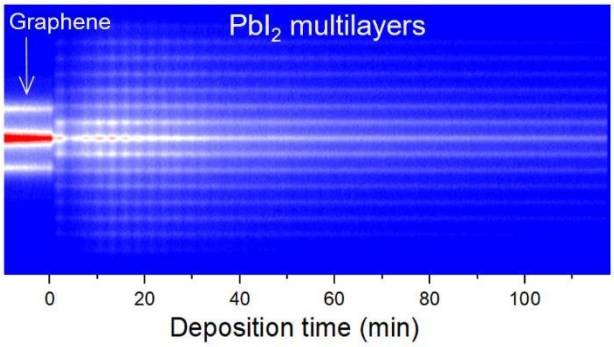

Fig. 1. Layer-by-layer growth of PbI_2 on graphene/SiC

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10. Epitaxial growth of MgO seed layers on R-plane sapphire substrates for enhanced perovskite oxide films for microwave applications

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The crystalline quality of functional thin films grown on Al_2O_3 single crystals (sapphire) is a critical factor for several applications at microwaves. To address this issue, introduction of seed layers is generally required to accommodate crystal structure mismatch between pseudo-cubic perovskites and rhombohedral-Al_2O_3. The present study focuses on the growth of MgO layers on $(1\bar{1}02)$-Al_2O_3 surface (R-plane sapphire) to provide suitable crystalline template for the subsequent deposition of ferroelectric $Ba_{0.7}Sr_{0.3}TiO_3$ (BST) thin films [1]. MgO thin films (15 to 50 nm-thick) were deposited on R-plane sapphire substrates by RF magnetron sputtering at various substrate temperatures (350 to 750°C) and characterized by X-ray diffraction (XRD) to investigate their growth mechanism. For all the samples, XRD $\omega - 2\theta$ scans aligned on the 012 sapphire peak show no contribution of the MgO layer (Fig. 1a), while $\omega - 2\theta$ scans aligned on the 002 MgO peak at $2\theta \approx 42.83°$ show an out-of-plane [002] texture with a tilt angle relative to the normal of the substrate surface ranging from 2° to 6° depending on substrate temperature. This tilted growth of MgO, previously reported in the literature, remains unexplained up to date [2]. Rocking curve analyses of the 002 MgO peak exhibit a narrowest full-width at half-maximum (FWHM) equal to 1.36° for the 50 nm-thick MgO seed layer grown at 550°C (related to a tilt of ≈ 4.8°), highlighting high crystalline quality (Fig. 1b). Pole figures of the {220} MgO planes (Fig. 1c) indicate an epitaxial relationship between MgO layer and sapphire substrate as follows: $(002)_{MgO}$ // $(012)_{Al2O3}$; $[100]_{MgO}$ //$[100]_{Al2O3}$; $[100]_{MgO}$ //$[\bar{1}\bar{2}0]_{Al2O3}$) and demonstrate an out-of-plane growth axis systematically tilted along the $[\bar{1}\bar{2}0]_{Al2O3}$ direction, such direction exhibiting the highest lattice mismatch with MgO (Fig. 1d). Based on the Domain Matching Epitaxy and Yamada's model [3-4], this study proposes a growth model supported by the reduction of atomic site mismatch at the MgO layer/sapphire interface through specific tilt of the [002] MgO growth direction at a suitable deposition temperature range. Finally, the dielectric properties of BST thin films (600 nm-thick) deposited by RF magnetron sputtering on sapphire substrates with and without MgO seed layer were retrieved at microwaves (10 GHz). Cube-on-cube epitaxial growth of BST film on optimized MgO seed layer led to clear improvement of their dielectric properties ($\varepsilon_r = 445$ and $\tan\delta = 0.13$) compared with those of a randomly oriented BST film grown on bare sapphire substrate ($\varepsilon_r = 290$ and $\tan\delta = 0.16$).

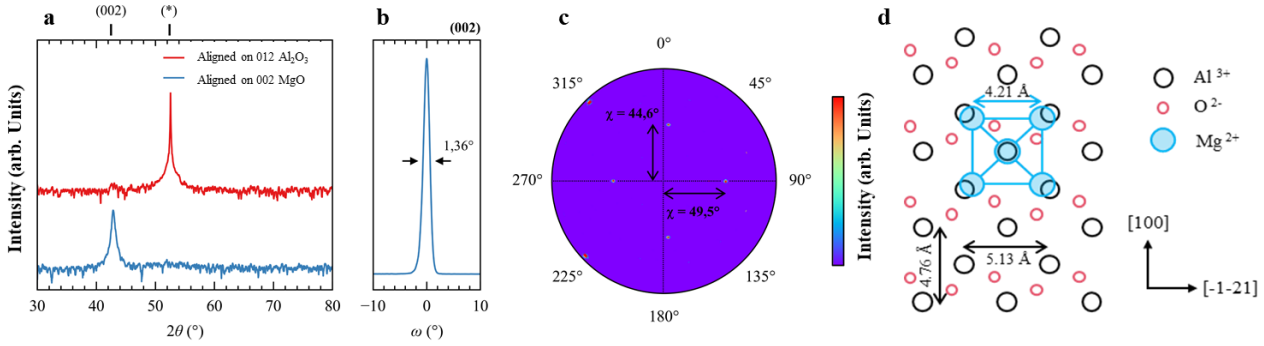

Figure 1: (a) XRD ω−2θ scans aligned on 012 Al_2O_3 and 002 MgO peaks, (b) Rocking curve of the 002 MgO peak, (c) Pole figure of the {022} MgO planes, and (d) schematic representation on the MgO seed layer growth on R-plane sapphire substrate.

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11. Evolution of the surface state of plastic cheese molds and its impact on Cheese/Mold adhesion: A physico-chemical and microscopic approach

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Cheese adhesion to plastic molds represents a major technological challenge in the cheese industry, affecting both productivity and demolding quality. This work aims to link the physical and chemical evolutions of mold surfaces to their adhesion behavior over their life cycle. Polypropylene molds, either new or subjected to various durations of use and cleaning, were characterized using Scanning Electron Microscopy (SEM), Fourier-Transform Infrared Spectroscopy (FT-IR) and contact angle measurements using 3 test liquids: water, diiodomethane, and ethylene glycol. Preliminary FT-IR analyses indicate the appearance of surface deposits after only a few weeks of use, suggesting the presence of protein, lipid [1] (and/or oxidation compound [2]), and lactose [3] deposits. SEM images reveal progressive surface heterogeneous deposits with use. These modifications are accompanied by variations in surface energy components, which may influence adhesion behavior. These findings contribute to a better understanding of cheese/mold interactions and open perspectives for optimizing cleaning processes and plastic material formulations.

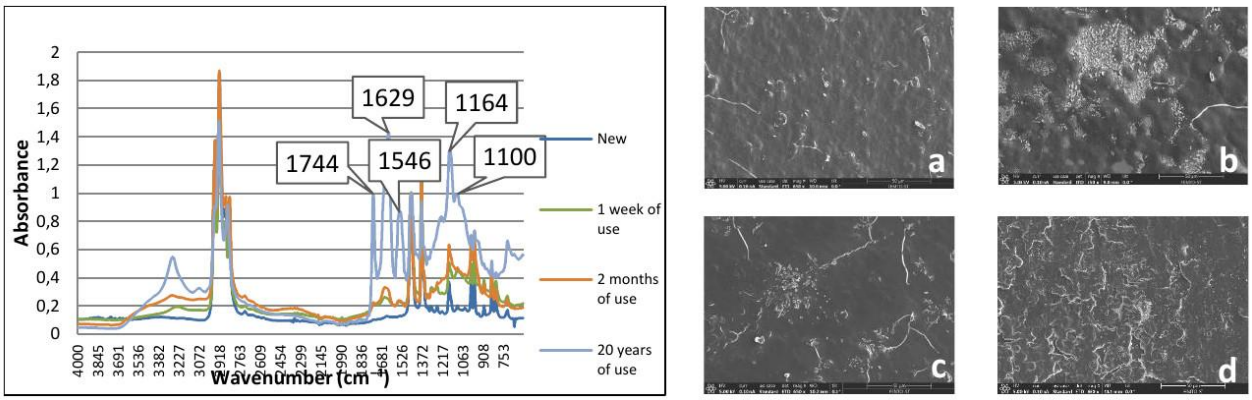

Figure 1. FTIR and SEM observations of polypropylene mold surfaces: (a) new mold, (b) after 1 week of use (c) 2 months of use (d) 20 years of use — surface deposits and topographical changes visible.

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12. Efficient Renormalization-Method Calculations of Angle-Resolved X-ray Photoelectron Spectra for Large-Scale Heterostructured Strontium

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Perovskite oxides (ABO_3) play a key role in emerging technologies such as spintronics, photovoltaics, and energy-efficient devices. They are particularly known for their dielectric properties and for unique interface phenomena, exemplified by the two-dimensional electron gas formed at the $LaAlO_3/SrTiO_3$ interface [1]. Because these properties originate from subtle atomic displacements near surfaces or interfaces, surface structural analysis is essential. X-ray photoelectron diffraction (XPD) is a powerful technique for this purpose. However, as the structural complexity of a material increases, XPD patterns become increasingly difficult to interpret. To address this challenge, numerical simulations are frequently employed. In this work, we simulated XPD spectra. One issue is that for large-scale perovskite clusters (~1000 atoms), the calculated XPD spectra diverge. Previous studies have proposed several “simple renormalization” schemes and demonstrated that such methods can suppress divergence in small clusters, such as 50-atom Cu clusters [2]. Applying these methods to perovskite systems, however, becomes computationally demanding, often requiring on the order of one month for a 1000-atom cluster.

To reduce the computational cost, we simplified the perovskite cluster into a one-dimensional atomic chain and applied one of the renormalization schemes to this reduced model. This approach was successfully validated for strontium titanate ($SrTiO_3$): the renormalized calculations showed excellent agreement with both MsSpec simulations and experimental XPD spectra (Fig. 1). Our results demonstrate that this renormalization-based 1D modeling approach can significantly accelerate XPD simulations for complex materials and may be extended to other oxide systems.

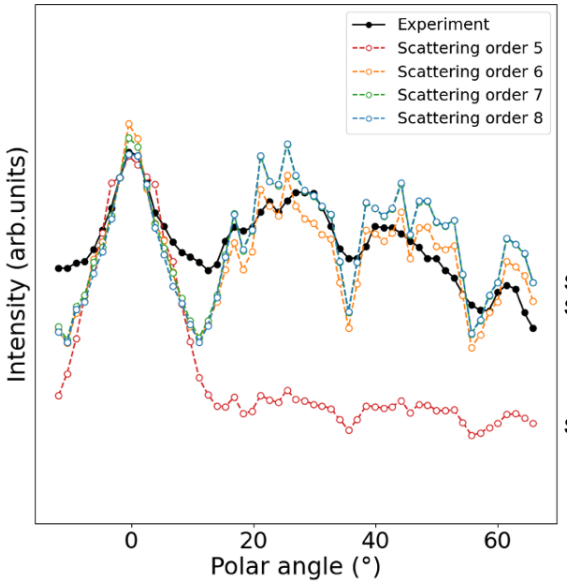

Fig.1: Simulation and Experiment.
Simulation has been performed by Series Expansion method with scattering order 5 ~ 8

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13. Improving Faradaic Efficiency for Conversion of Bicarbonate to Formate Using Bismuth-Indium Decorated Silicon Photocathodes

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Efficient CO_2 photoelectroreduction requires cocatalysts that not only provide active sites but also enable selective extraction of photogenerated electrons from the semiconductor. Here, we demonstrate that integrating bismuth-indium (Bi-In) metal nanostructures with silicon micro-pyramidal photocathodes markedly enhances both activity and selectivity for CO_2 to formate conversion. The Bi-In cocatalyst was deposited via a controlled electrodeposition process, allowing precise tuning of nanostructure morphology and surface coverage through the transferred charge. Compared with Bi only modified electrodes, Bi-In /Si photocathodes exhibit substantially higher formate production, reaching a Faradaic efficiency of 90% at −1.0 V versus the reversible hydrogen electrode. Experimental characterization indicates that favourable band alignment at the Bi-In /Si interface facilitates photogenerated electron transport and selectively promotes the CO_2-to-formate reaction pathway. These results establish dual metal cocatalyst engineering as an effective strategy for controlling interfacial charge transport and reaction selectivity in photoelectrocatalytic CO_2 reduction.

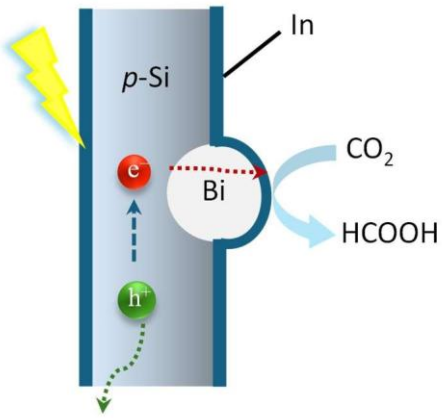

Fig.1. Proposed mechanism for photoelectrochemical CO_2 reduction on the Bi-In /Si photocathode.

14. Embedded cobalt nanoparticles for combined magnetic and thermoelectric properties

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Interface effects are known to play a major role on the transport properties (charge and heat) of nano-composites [1]. Here we will present an investigation of the thermoelectric properties of a semiconducting thin film where Cobalt nanoparticles have been embedded with a low concentration (a few atomic %), resulting in an assembly of nanomagnets behaving as “macrospins” [2]. Motivated by recent results [3], our objective is to study the effect of such nanomagnets, as well as the influence of the overall magnetic state, on the electrical and thermal transport coefficients. Our nano-composite system is composed of a germanium matrix grown simultaneously to the co-deposition of preformed clusters using the Low Energy Cluster Beam Deposition method (LECBD [2]) under ultrahigh vacuum conditions.

In the frame of the French ANR project called ENATHER, where we want to modify the thermoelectric properties using embedded nanomagnets of adjustable size, concentration and magnetic configuration, we have been able to produce samples with preserved Co nanomagnets in amorphous germanium (see Fig. 1), displaying the expected blocked-superparamagnetic crossover. We observe that the inclusion of Co particles has a drastic impact on the electronic conductivity (see Fig. 1) while the Seebeck coefficient shows a strong phonon drag peak at low temperature. The inclusion of metallic macrospins in a semiconducting material results in a complex system where many physical phenomena are involved (interface diffusion, charge and phonon scattering, doping & charge transfer, spin polarization, magnetic interactions etc.) and the question of a magnetic signature on the transport properties in this kind of system is still open. The preliminary results we show illustrate the new line of investigation of our “Transport, nanomagnetism and materials for energy” team, devoted to the transport properties (charge and heat) and their coupling with magnetism in nano-systems.

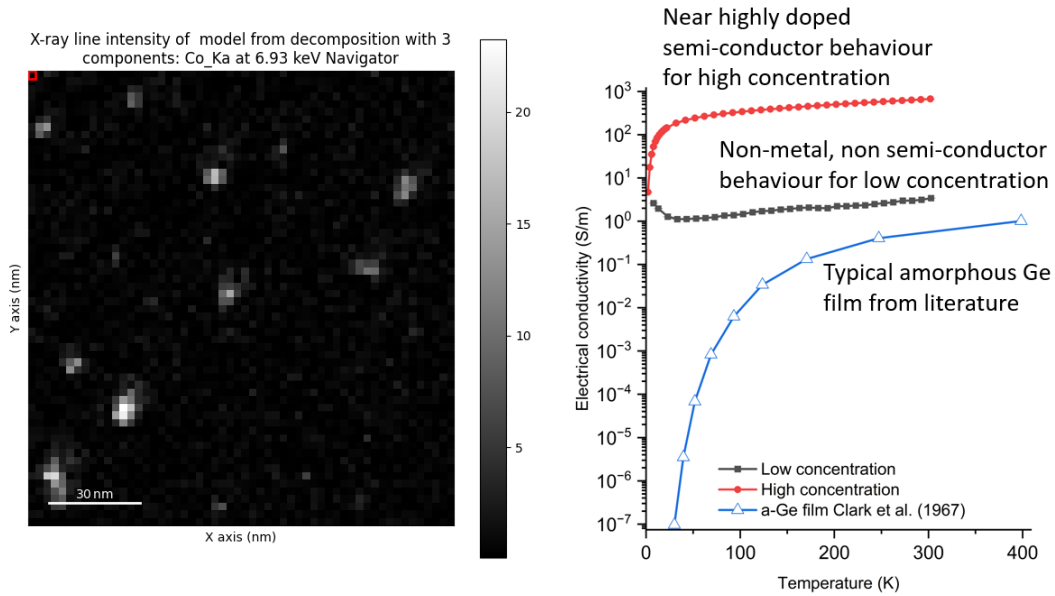

Fig.1. STEM-EDS observation (left) and electrical conductivity (right) of Co@Ge nano-composite thin films.

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15. Propriétés physico-chimiques et propriétés électroniques de pérovskite 2D $Ca_2Nb_3O_{10}$ à haute permittivité diélectrique déposée sur silicium

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Les pérovskites suscitent un intérêt fondamental et appliqué considérable du fait de leur large spectre de fonctionnalités physiques, allant de propriétés diélectriques, ferroélectriques, ferromagnétiques et piézoélectriques remarquables jusqu'à la supraconductivité et la magnétorésistance colossale. L'intégration de ces matériaux en couches minces nécessite des méthodes de croissance complexes (ablation laser pulsée, épitaxie par jets moléculaires) incluant souvent un recuit post-dépôt à haute température (>600°C) favorisant la réactivité aux interfaces et la génération de défauts cristallins induits notamment par la contrainte thermique. Dans ce contexte, l'exfoliation chimique de pérovskites lamellaires de type Dion-Jacobson permet la mise en œuvre de dépôts couche par couche, homogènes sur de grandes surfaces, via une méthode de type Langmuir-Blodgett (LB) à budget thermique nul [1].

Dans cette communication nous présentons une étude du transfert de monofeuillets $Ca_2Nb_3O_{10}$ sur une surface de silicium en vue de leur intégration comme isolant à forte permittivité diélectrique (ε_r=200) [2] dans des structures MOS (metal-oxide-semiconductor). Des monocristaux de la phase Dion-Jacobson $KCa_2Nb_3O_{10}$ ont été préparés par réaction à l'état solide à partir de précurseurs de K_2CO_3, Nb_2O_5 et $CaCO_3$. Dans les cristaux obtenus, les ions potassium sont d'abord échangés par des protons en milieu acide. L'exfoliation chimique des nanofeuillets de $Ca_2Nb_3O_{10}$ est ensuite obtenue en substituant aux protons des ions tétrabutylammonium massifs permettant la délamination de la structure [3]. La solution colloïdale de nanofeuillets obtenue est finalement utilisée pour des dépôts LB sur substrat de silicium présentant un oxyde natif en surface. Dans un premier temps, nous démontrons par spectroscopie de photoélectrons X (XPS) que les traitements chimiques conventionnels permettant de nettoyer la surface du silicium en microélectronique n'affectent pas les nanofeuillets pérovskites déposés, ouvrant ainsi la voie à leur intégration sur ce substrat. Dans un second temps, nous avons étudié conjointement par XPS et microscopie à effet tunnel (STM) la stabilité thermique des nanofeuillets. Si les feuillets n'évoluent pas lors d'un recuit sous ultravide à 160°C, nous démontrons la formation de lacunes d'oxygène en surface des nanofeuillets à 400°C associée à une réduction partielle des atomes de Nb. Cet effet est parfaitement réversible par recuit à 100°C à l'air. Enfin nous avons réalisé des structures MOS $Au/Ca_2Nb_3O_{10}/Si$ et étudié leurs propriétés électroniques locales par microscopie à émission d'électrons balistiques [4]. Les mesures ponctuelles locales à la verticale d'un nanofeuillet démontrent une hauteur de barrière tunnel de 1.5 eV à l'interface $Au/Ca_2Nb_3O_{10}$. L'étude des propriétés électriques des MOS intégrant un monofeuillet constitue la perspective naturelle de ce travail. Nous envisageons également l'intégration de ces barrières tunnel modèles (rugosité nulle) dans des jonctions tunnel magnétiques épitaxiées.

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16. Plasmons and electronic excitation spectrum of gold (111) surface with time dependent density functional perturbation theory including Hubbard's U

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Surface plasmons offer the possibility of light confinement in regions close to the surface, and have a variety of applications in biology, physics and medicine, for instance for trace analysis with surface plasmon (SP) resonance spectroscopy, or to increase the efficiency of energy harvesting in solar cells. They have also been studied recently by Time-Resolved and Ultrafast Electron Energy-Loss Spectroscopy [1].

The theoretical study of such surface response functions (loss function, or imaginary part of the inverse dielectric function), is mandatory to obtain the correct interpretation of the spectral information obtained experimentally. In the present work we revisit the important case of the gold (111) surface by theory and experiment, using TDDFPT+U as implemented recently in TURBOEELS [2,3] a well has high resolution electron energy loss spectroscopy (HREELS) experiments [4] . Inclusion of intraband Coulomb interaction through DFT+U in the 5*d* electronic band has proven to be crucial to obtain the proper positioning, with respect to the plasmon energies, of interband transition band energies coming from the 5*d* states.

Calculations have been performed with the Quantum TURBOEELS codeand the ESPRESSO software. We use the implementation of ultrasoft pseudopotentials tested for bulk gold [5]. Access to high performance computing (HPC) resources have been granted by the IDRIS, CINES, TGCC national centers (GENCI Project 2210 and TGCC special allocation), and by the Partnership for Advanced Computing in Europe (Project 2010PA3750). We acknowledge support from the ANR BCSi project.

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

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

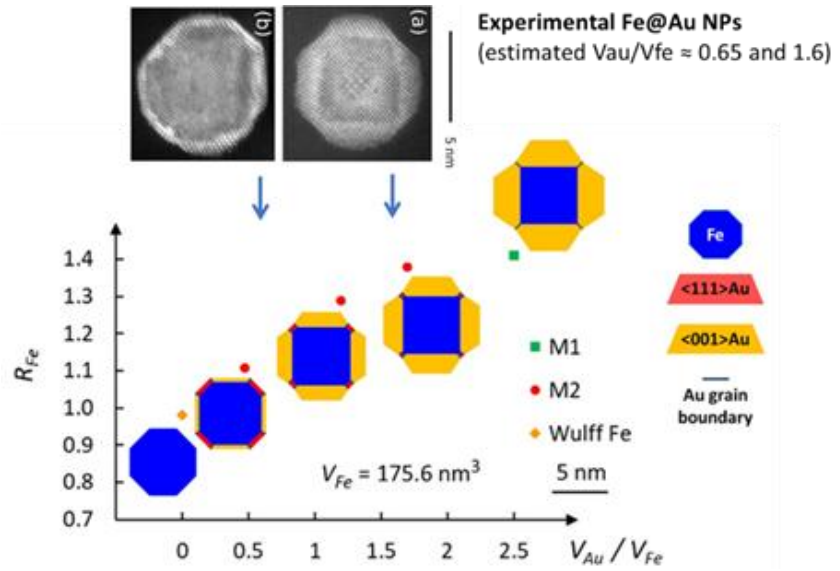

Fig.1 : Evolution of the equilibrium shape of Fe@Au nanoparticles, as a function of the Au/Fe volume ratio [2].

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18. Symmetry and morphology of bcc@fcc core@shell metallic nanoparticles drived by epitaxial relationships at bcc-fcc interfaces

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

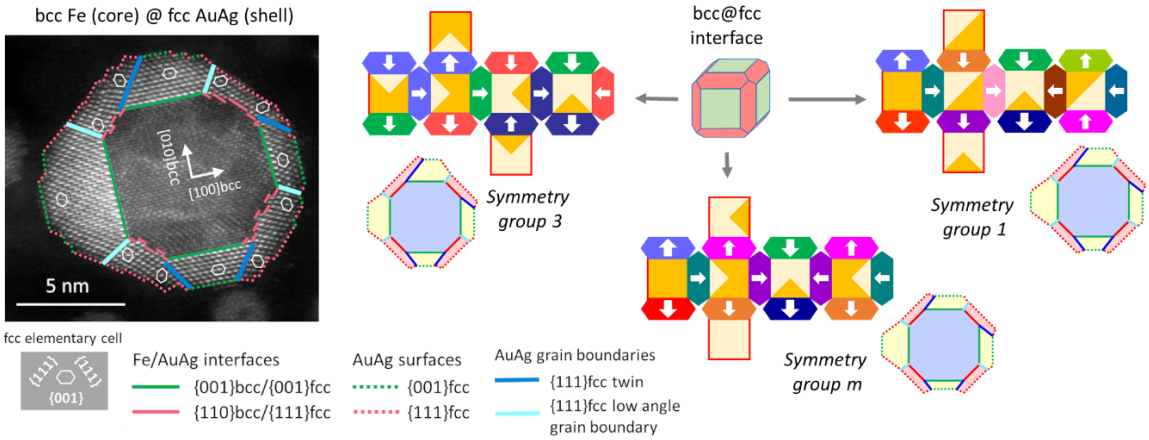

Fig.1 : Crystallographic analysis of a Fe@AuAg NP, observed along a <001> direction of the Fe core, and scheme of some possible 3D morphologies for this NP [4].

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

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19. Electrode-induced strain redistribution in epitaxial ferroelectric LSMO/BTO/LSMO heterostructures grown on $SrTiO_3$ substrates.

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Strain engineering in epitaxial thin films is of great interest, as it enables the tuning of functional properties. In ferroelectric materials this is of pivotal interest, strain can modify the amplitude, orientation, and switching behavior of the electric polarization [1], [2], [3]. However, the use of conductive electrodes required for electrical measurements may strongly influence the strain state during growth, leading to unexpected structural distortions and electrical measurements drifts.

To investigate this effect, four $La_{0.67}Sr_{0.33}MnO_3$ (LSMO) / $BaTiO_3$ (BTO) and LSMO/BTO/LSMO heterostructures were fabricated by combining pulsed laser deposition (PLD) and oxygen-assisted molecular beam epitaxy (OA-MBE). A 12 nm LSMO bottom electrode was first grown by PLD on (001)-oriented $SrTiO_3$ substrates, followed by BTO layers of 5, 8, 17, and 24 nm deposited by OA-MBE. X-ray diffraction (XRD) measurements were performed both, before and after deposition, of a 15 nm LSMO top electrode to track the strain evolution within the heterostructures.

The XRD patterns confirm highly oriented [001] epitaxial growth with Laue oscillations, indicating smooth interfaces, coherent growth and high crystalline quality. Depth-resolved fitting of 2θ/ω scans, achieved by modeling each layer as several sublayers (3–5 nm thick), reveals a clear strain gradient through the heterostructure (Fig. 1). The LSMO bottom electrode exhibits compressive out-of-plane strain near the STO substrate that gradually relaxes toward the BTO interface, where it becomes slightly tensile due to the positive lattice mismatch. In the as-grown state (without top electrode), the 5 nm BTO film remains coherently strained, while thicker layers progressively experience strain relaxation with lattice parameter evolving toward bulk-like parameters. After deposition of the top LSMO electrode, a strong redistribution of strain occurs: the BTO layer undergoes a transition from tensile to compressive out-of-plane strain, induced by the negative in-plane mismatch with the upper LSMO. The top electrode itself displays compressive out-of-plane strain followed by partial relaxation near the surface.

These results demonstrate the crucial influence of the top electrode on strain distribution in ferroelectric heterostructures. Complementary RHEED and cross-sectional TEM analyses are currently being performed to further resolve the interfacial structure and strain relaxation mechanisms.

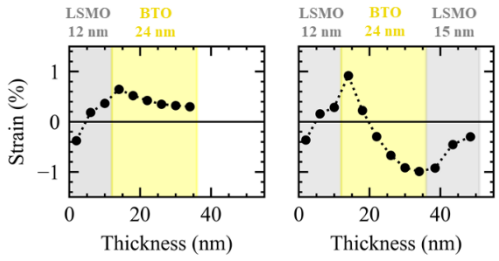

Fig.1. Depth-resolved strain into the LSMO/BTO and LSMO/BTO/LSMO heterostructures extracted by fitting the 2θ/ω scans.

This research was funded by the French National Research Agency under project ANR-23-CE42-0011 (POLARYS)

[1] J. H. Haeni *et al.*, *Room-temperature ferroelectricity in strained $SrTiO_3$*, Nature 430 (2004), p. 758-761.
[2] J. Tu *et al.*, *Giant switchable ferroelectric photovoltage in double-perovskite epitaxial films through chemical negative strain*, Sci. Adv. 11 (2025).
[3] D. Sando, *Strain and orientation engineering in ABO_3 perovskite oxide thin films*, J. Phys. Condens. Matter 34 (2022), p. 153001.

20. Enhancing Ferroelectric and Optoelectronic Thin Film Properties: The Role of 2D Oxide Nanosheets and Substrate Engineering

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Integration on low-cost substrates such as silicon or glass of high-quality perovskites thin films with enhanced properties remains a significant challenge in electronics and optoelectronics. These last years, oxide nanosheets (NS) have emerged as a promising solution to this challenge. NS facilitate improved structural and electrical properties in thin films [1]. In this study, we focus on the deposition of oxide NS, such as $[Ca_2Nb_3O_{10}]^-$ and $[Ti_{0.865}O_2]^{0.54-}$[2], onto various substrates (Fig. 1a), including glass, platinized silicon or textured silicon (Fig. 1c). By utilizing the distinct properties of these different substrates, we aim to improve the structural quality and performance of thin films, such as $K_{0.5}Na_{0.5}NbO_3$ (KNN), $SrVO_3$ and $SrNbO_3$.

Currently, lead zirconate titanate piezoelectric thin films are widely used in microelectromechanical systems. However, due to environmental concerns related to lead, research has shifted towards lead-free alternatives like KNN Since piezoelectric behavior varies with crystal orientation, polycrystalline films show inferior piezoelectric performance compared to oriented films. In this research, by using NS as seed layer, KNN thin films show enhanced crystalline orientation (Fig. 1b), suggesting improved performance. This enhancement has been described in earlier work by reducing defect densities [3]. In addition, indium tin oxide is widely used as transparent conducting oxides (TCOs) in displays and solar cells, the scarcity and possible volatility of indium costs makes it necessary to look for sustainable alternatives. Oxide perovskites, such as $SrVO_3$ or $SrNbO_3$, are very promising as TCOs with excellent performance not only in the visible spectrum but also extend into the ultraviolet range, making them suitable candidates for a variety of optoelectronic applications. Since their properties depend on their crystallization which can be difficult to obtain directly on glass [4], the use of NS as seed layers facilitates nucleation and growth of these materials, their optimizing their functional properties [1].

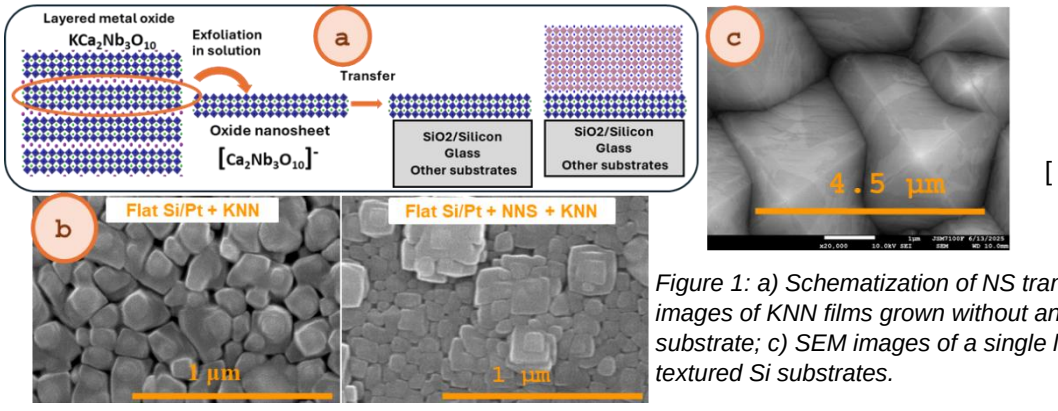

Figure 1: a) Schematization of NS transfer onto substrate; b) SEM images of KNN films grown without and with NS on a Pt/Si substrate; c) SEM images of a single layer of $[Ti_{0.865}O_2]^{0.54-}$ NS on textured Si substrates.

The authors acknowledge the French “Agence Nationale de la Recherche ANR” in the framework of the TILPAC project (ANR-22-CE08-0017), DisTCOvery project (ANR-23-CE08-0008) and Solstice project (ANR-22-PETA-0011) for financial support.

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21. Interpretable Machine Learning Connects Electronic Structure Models to Adsorption on N-Doped Graphene Single-Atom Catalysts

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Among the various models used to describe catalytic activity, the d-band model is well-established and widely applicable to numerous catalytic systems [1]. However, its predictive power decreases in the context of single-atom catalysts due to the molecular character of these systems, which display atomic-like d-states. In this work, based on interpretable machine learning, we demonstrate that the d-band model can be effectively extended to 3-fold coordinated transition metals in nitrogen-doped graphene single-atom catalysts (Fig. 1) [2]. The contribution from the support sp-states is significant and attractive, and it depends on both the atomic number of the transition metal and the number of its nitrogen neighbors. The contribution from the support d-states is mediated through the d-band center. Our model is applied to predict the reaction energy of selective butadiene hydrogenation, yielding mean absolute errors of 0.18 eV and 0.14 eV for the training and test sets, respectively. This approach opens new avenues for the rational design of high-performance single-atom catalysts, where the interplay between dopants, support interactions, and orbital contributions can be systematically tailored to enhance catalytic efficiency in selective hydrogenation and other critical reactions.

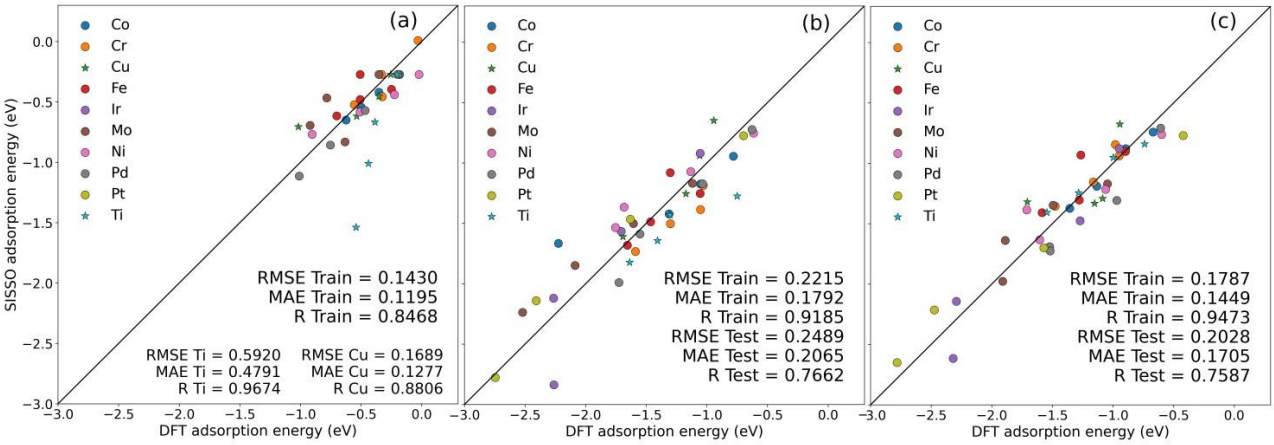

Fig. 1 : Parity plots for adsorption energies (dim 2, rung = 1) of both train set (circles) and test set (stars). (a) H_2, (b) butadiene and (c) butene.

[1] Hammer, B.; Norskov, J. K. Why gold is the noblest of all the metals. Nature 1995, 376, 238–240.
[2] Bequet, T ; Ziat, S., Brix, F., Gaudry, É Interpretable Machine Learning Connects Electronic Structure Models to Adsorption on N-Doped Graphene Single-Atom Catalysts, submitted

22. Engineering the MoS_2/Au Interface via Intermetallic Alloying: Weakening of Covalent-Like Quasi-Bonding in Exfoliated Monolayers

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Recently, the metal-assisted exfoliation of transition-metal dichalcogenides (TMDs) has emerged as a promising method for producing large-area, high-quality monolayers (MLs) thanks to the covalent-like quasi-bonding (CLQB) interaction at the interface between the first TMD layer and the metal substrate. This noble metal-assisted exfoliation method has been demonstrated for more than 40 different layered materials [1], opening up a new area for systematic studies of the richness of the electronic phases of the TMDs at the single layer limit. However, although this method allows record lateral sizes to be obtained, the very strong coupling at the TMD/metal interface drastically alters both the atomic and electronic properties expected for a free-standing ML, and further prevents the elaboration of twisted TMDs heterostructures using the 'tear and stack' method. 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 CLQB interaction at the TMD-Au interface by controlling the formation of an intermetallic $AuAl_2$ alloy using Al as adhesion layer with 1:2 atomic ratio and annealing procedure in a controlled atmosphere [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 ML. 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 $AuAl_2$ intermetallic alloy resulting in a strongly weakened CLQB interaction at the MoS_2 ML/metal interface.

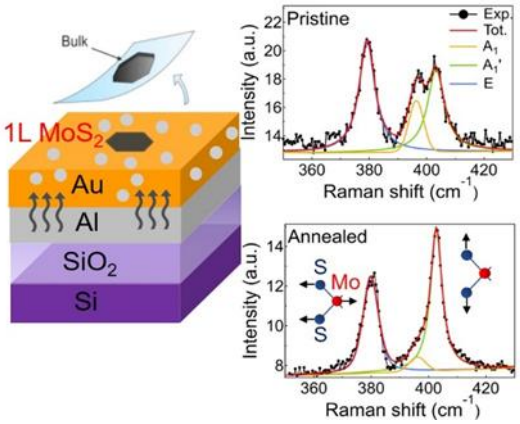

Figure 1. Left-hand side: Schematic drawing of the used experimental procedure for decoupling a large-area TMD monolayer that was exfoliated on Au. Right-hand side: Raman spectra of MoS_2 monolayer supported on Au before (pristine) and after annealing (annealed).

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23. Utilisation de solvants eutectiques profonds (DES) comme surfaces actives bioinspirées dédiées à la détection de CO_2 dans un système hyperfréquence

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L'objectif de ce travail de thèse est le développement de capteur de gaz couplé à un système hyperfréquence (quelques GHz). La couche sensible liquide est constituée d'un solvant eutectique profond (DES). La détection concerne les modifications des caractéristiques diélectriques de cette couche, ce qui influe directement sur la fréquence de résonance d'un stub ouvert en circuit imprimé. Le capteur permet de montrer une détection de l'effet de la solubilisation de CO_2 dans le DES.

En effet, les solvants eutectiques profonds (DES) obtenus par l'association de deux ou plusieurs composants qui forment un mélange ayant un point de fusion significativement plus bas que celui de chacun des constituants pris individuellement [1]. Ils sont généralement constitués d'un donneur et d'un accepteur de liaisons hydrogène, ce qui leur confère des propriétés physico-chimiques particulières adaptées pour des processus d'extraction et de purification, comme catalyseur ou solvant dans des synthèses organiques. Les solvants eutectiques profonds (DES), et en particulier les NADES (Natural Deep Eutectic Solvents) formulés à partir de constituants d'origine biologique (sucres, acides organiques, acides aminés, …), offrent une plateforme verte et fortement modulable pour la capture et la solubilisation de gaz tels que CO_2 [2][3]. L'étude porte sur plusieurs DES et leur sensibilité au bullage de différents gaz.

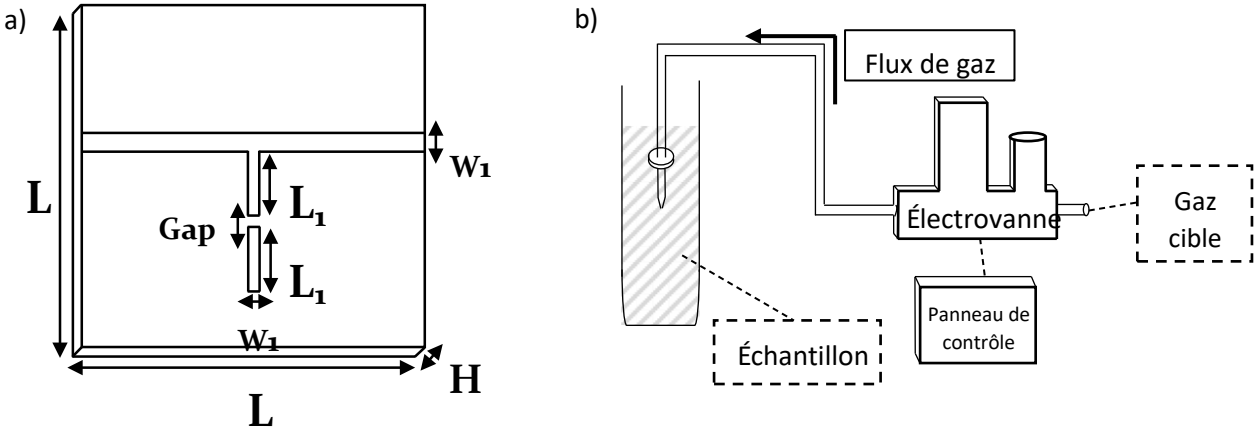

Fig.1.a) Représentation schématique du dispositive hyperfréquence (résonateur a stub ouvert), b) Représentation schématique du dispositif de bullage de CO_2 dans un échantillon de DES.

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[2] S. Sarmad, Y. Xie, J.-P. Mikkola, et X. Ji, « Screening of deep eutectic solvents (DESs) as green CO2 sorbents: from solubility to viscosity », *New J. Chem.*, vol. 41, nº 1, p. 290-301, déc. 2016

[3] E. Ali *et al.*, « Solubility of CO2 in deep eutectic solvents: Experiments and modelling using the Peng–Robinson equation of state », *Chemical Engineering Research and Design*, vol. 92, nº 10, p. 1898-1906, oct. 2014,

24. Direct observation of edge states in plumbene using Scanning Tunneling Microscopy

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Since the discovery of graphene, research on 2D materials in general and particularly honeycomb structure, has attracted significant attention. The topological properties in these lattices strongly depends on spin orbit coupling (SOC) [1]. SOC induces a band gap around the Dirac point, while giving rise to linearly disperse gapless edge states [2]. Plumbene is a monolayer of Pb where hexagonally arranged Pb atoms form honeycomb structure similar to graphene. Due to high atomic number (Z) of Pb, it can possess significant topological properties such as topological edge states [3]. However, the synthesis of plumbene is challenging as it requires suitable substrate compatibility and control over the growth conditions [4]. In this work, we have identified 6H-SiC(0001) sample as a suitable substrate and demonstrate that one of the surface reconstruction promotes the growth of Pb honeycomb lattice, which has been confirmed with surface diffraction. Low energy electron diffraction (LEED) reveals a clear 2×2 superstructure, which is further confirmed with scanning tunneling microscopy (STM). Scanning tunneling spectroscopy (STS) reveals presence of electronic states localized at the domain boundaries, similar to edge states. Remarkably, similar spectroscopic features are anticipated to emerge at a single-atom vacancy domain, suggesting that atomic scale defects can host localized topological edge states. A detailed analysis of this features is currently underway. These findings provide experimental evidence of topological edge states of a substrate supported plumbene.

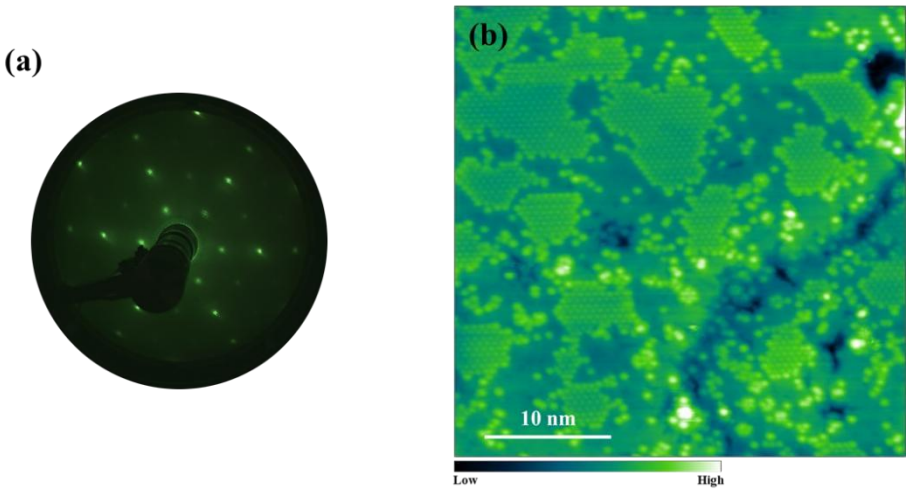

Figure 1. (a) LEED pattern is showing 2×2 superstructure of Pb, taken at 122 eV, (b) STM image of the Pbdomains. Tunnelling conditions: V= -2.5 V, I= 40 pA, T= 77K.

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[4] Yong Han et al., *J. Phys.: Condens. Matter* **37** 373001 (2025)

25. Higher order topological defects in the moiré lattice of a van der Waals magnetic material

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Van der Waals materials are emerging as extremely versatile building blocks for many fields of research, both at the fundamental and applied level. They offer tremendous possibilities for fine tuning spintronics, superconducting, nanoelectronics, optical devices. They appear extremely attractive for exploring new exotic physics due to their ability to be staked with an infinite number of combinations that leads to unexpected physical properties. The toolbox of van der Waals heterostructures is continuously growing with for instance the recent discovery of ferromagnetic order down to the monolayer limit in the family of chromium trihalide, $CrCl_3$, $CrBr_3$ and CrI_3 (CrX_3, X= I, Br, Cl) [1]. Several works have related some observations of moiré structure due to the mismatch between the CrX_3 monolayers and their substrate which lead to a wealth of new exotic effects [2, 3]. Combining a chromium trihalide layer with a superconductor might lead for instance to topological superconductivity as recently reported in $CrBr_3/NbSe_2$ heterostructures [4]. In this hybrid structure, it was proposed that the mechanisms leading to a topological order in this hybrid structures was intimately related to the presence of a moiré pattern [2]. Another fascinating observation is about the influence of a moiré on the magnetic properties. In the CrX_3 family, till now, the magnetization was shown to be essentially colinear, however, in CrI_3 double bilayer some hint of non-colinear magnetism was found and was related to the moiré pattern which leads to a non- negligible spatial modulation of the magnetic interaction [3]. In this communication I will present our scanning tunneling microscopy investigation of a $CrCl_3$ monolayer deposited on Au(111) which exhibit a second order moiré pattern. We report the presence of edge dislocations in this moiré pattern (see figure). Based on a comprehensive analytical model, I will show that these well know edge dislocations can be reexamined in the framework of topological concepts where they are described as topological defects analogous to vortices carrying a Berry phase characterized by a Chern winding number. They might therefore be use as a pinning center to host topological spin texture and / or Majorana bound states in CrX_3/superconductor heterostructures.

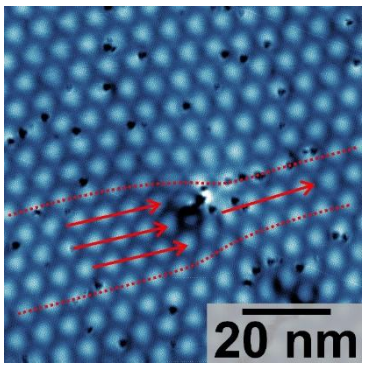

Figure: Edge dislocation in the moiré pattern formed between $CrCl_3$ monolayer and Au(111). It exhibits a Burger vector 2 times larger that the moiré unit cell.

[1] D. Soriano et. al, Nano Lett. 20, 6225 (2020)
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[4] S. Kezilebieke et. al, Nature 588, 424 (2020)

26. Cost-effective Ni-based catalytic electrodes for alkaline (sea)water splitting

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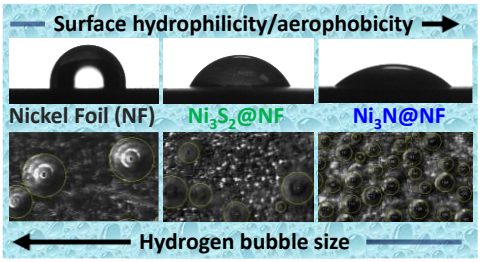
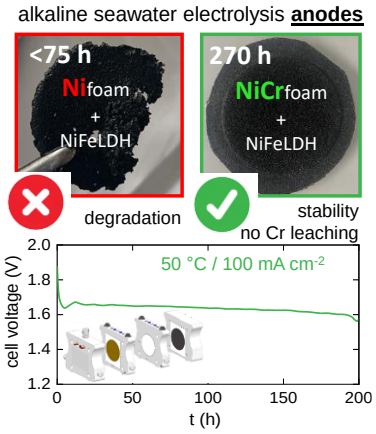
Dihydrogen (H_2) is considered nowadays as a sustainable energy carrier and exhibits a high energy density in its highly compressed state [1]. Different countries in the world are developing industrial production and are scaling up water electrolysis processes with clear roadmaps [2]. Alkaline water electrolysis is an affordable technology that avoids the use of platinum group metals with a good compromise of efficiency because of the development of new cost-effective and Earth-abundant materials of electrodes and new anion-exchange membranes [3,4].

We present our recent results on single-phase nickel nitride (Ni_3N) and nickel sulfide (Ni_3S_2) hydrogen evolution reaction (HER) electrocatalysts which were grown directly on a flat nickel foil (NF) using a simple and original approach. The electrode Ni_3N@NF showed the best HER activity in 1M KOH, in terms of onset potential and overpotential at 10, 100 and 200 mA cm^{-2}. Combining electrochemical measurements with in situ bubble dynamics study and DFT calculations, we demonstrate that the superior catalytic activity of Ni_3N compared to Ni_3S_2 for alkaline HER can be attributed to its more hydrophilic character leading to smaller electrogenerated H_2 bubbles and shorter retention time on the electrode [5].



We also show that the assembly combining highly active NiFe layered double hydroxyde (LDH) electrocatalyst with novel alloyed NiCr foam anodes exhibits high corrosion resistance during alkaline seawater electrolysis (ASE), minimal Cr leaching in the electrolyte and long-term efficiency [6]. An ASE electrolyzer comprising the so-prepared anode and a cathode derivatized with $NiMoO_4$ was stable in operation at 50°C for 270 h at a current density of 100 mA cm^{-2} and a Ohmic drop-corrected voltage of 1.6 V. These results open opportunities for direct seawater electrolysis and evidence the synergistic interplay between the electrode support and the oxygen evolution reaction (OER) electrocatalyst for improving anodic lifetime at high current densities in alkalinized seawater [7].



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27. Impact de la dynamique de bulles sur l'électrolyse de l'eau

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Une difficulté dans le développement de la production de dihydrogène par électrolyse tient à la présence des bulles de H_2 et de O_2 qui interagissent, via leurs dynamiques, et affectent ainsi la pureté des gaz produits. Le défi posé par l'électrolyse sans membrane consiste à séparer les gaz de l'électrolyse sans utiliser de séparateur physique. Une solution consiste à ajouter un flux permettant l'évacuation des gaz produits, réduisant ainsi le rendement global de l'électrolyseur. Notre approche consiste à comprendre les propriétés et effets de la dynamique des bulles sur l'électrolyse afin d'aider à la conception d'électrolyseurs sans membrane. A cette fin, nous proposons une approche numérique qui couple cycle de vie d'une bulle (nucléation et détachement [1,2], dynamique [3]) et mesure électrochimique. Ce méta-modèle nous permet à la fois d'accéder à des mesures locales (rayon de détachement des bulles tenant compte des interactions hydrodynamiques entre bulles, cartographie du potentiel et de la densité de courant) et globales (quantité de dihydrogène produit, surtension, zone occupée par les bulles en interaction…). La figure ci-dessous illustre une cartographie de potentiel obtenue ainsi que la surtension de notre électrolyseur pour différentes densités de courant appliquées. Durant la présentation, nous exposerons les points clés des modèles utilisés, et insisterons davantage sur les résultats que nous pouvons obtenir, ainsi que sur la polyvalence de notre approche.

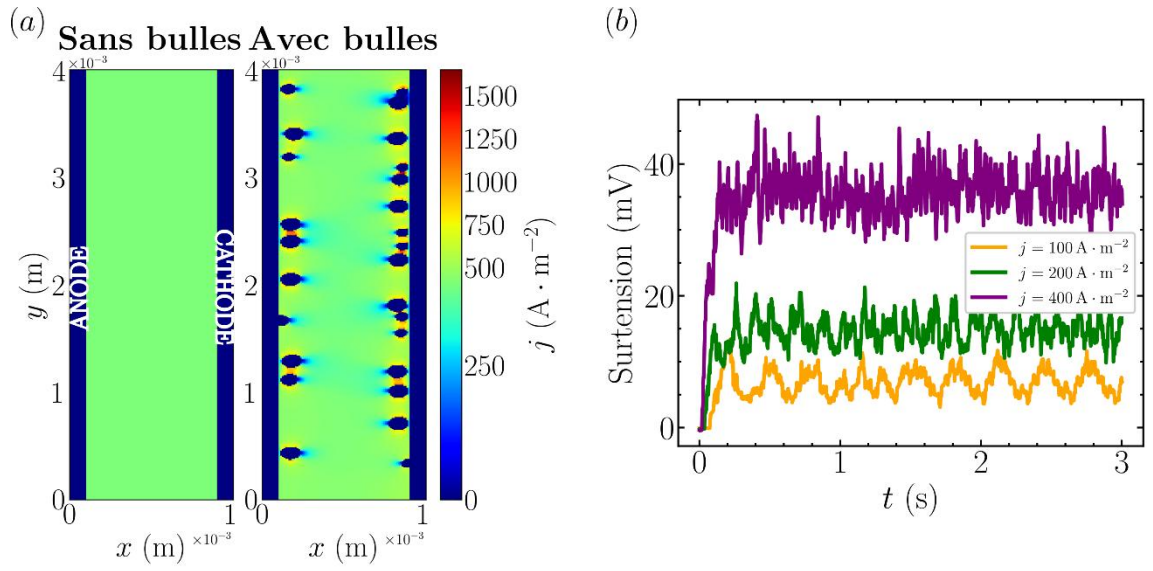

Figure : a) Cartographie de la densité de courant dans l'électrolyseur (les électrodes sont indiquées en bleu foncé) sans et avec bulles pour une densité de courant appliquée de 400 A.m^{-2}, b) Surtension globale en fonction du temps pour différentes densités de courant appliquées, en présence de bulles.

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28. Propriétés structurales et électroniques de couches ultra-minces de bismuth à la surface de l'Au(111)

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La découverte du graphène a suscité un intérêt majeur dans le domaine des matériaux 2D, notamment du fait de la mobilité exceptionnelle de ses porteurs de charge liée à sa structure bidimensionnelle. Dans ce cadre, l'obtention de couches ultra-minces de bismuth (Bi) ayant un fort couplage spin orbite, contrairement au graphène, ainsi que des propriétés topologiques originales est apparue comment particulièrement prometteuse. Des calculs rapportés dans la littérature montrent un diagramme de phase extrêmement riche pour le Bi 2D [1]. Parmi ses phases métastables, le α-bismuthène se distingue par ses propriétés électroniques remarquables. Il a été synthétisé sur des substrats tels que le HOPG, le SnSe ou encore le SnS. Par ailleurs, la croissance des films minces de Bi a aussi été réalisée sur des métaux nobles comme l'Au(111) [2], dont l'étude des propriétés électroniques reste très limitée. Dans ce travail, nous nous sommes intéressés à la croissance et l'étude des propriétés structurales et électroniques de couches ultra minces de Bi sur l'Au(111) dans le régime de quelques monocouches. La croissance des couches ultra minces de Bi sur Au(111) présente une succession de phases complexe. Dans le régime sous la monocouche, deux phases ordonnées apparaissent successivement : (i) une première structure hexagonale notée $\sqrt{37} \times \sqrt{37}R25.3°$ et (ii) une seconde structure rectangulaire notée $p \times \sqrt{3}$, associée à un Moiré, et dont la structure de bandes est particulièrement visible à basse énergie (états 6p du Bi) (Figure 1). A plus haut taux de couverture, la croissance conduit à la phase α-bismuthène. Dans ce travail, nous présenterons nos résultats obtenus sur ces différentes phases, notamment l'évolution des propriétés structurales par LEED et STM. Nous discuterons également l'évolution des propriétés électroniques obtenues par ARPES et STS haute résolution.

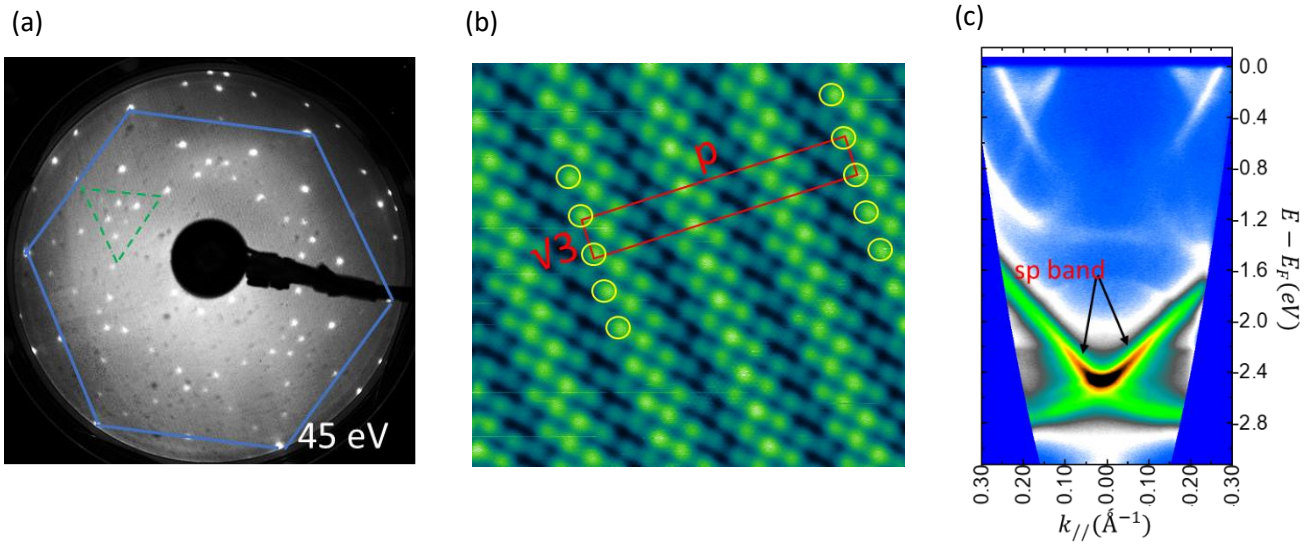

Figure 1 : Propriétés structurales et électroniques du Bi/Au(111) : illustration pour la phase $p \times \sqrt{3}$ avec p=5. (a) cliché LEED pris à 45 eV, (b) image STM (6nm²) et (c) spectre ARPES (hv=8.44eV).

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29. Electronic Fabry Perot interferometer as a model to describe electron confinement in ultrathin films of Pb on Ag(111)

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Many studies report on electron confinement in thin metallic films, experimentally and theoretically as well [1-4]. In most of the cases, the energy of the quantum resonances that develop in the film can be predicted from the simple model known as “Phase Accumulation Model” (PAM). In this model the confined electrons accumulate phase shift not only due to the propagation in the film (leading to the thickness dependence of the phase) but also due to their reflections both at the surface of the film and at the interface between the film and the substrate. The latter phase shifts are both energy dependent, making the energy of the quantum resonances sensitive to the surface and interface properties. If a graphical solution of the PAM permit to predict the resonance energies, the full spectrum of resonances obtained from STS measurement can be simulated by using a Fabry Perot Model (FP) adapted to electrons [1]. In this communication we will compare the measured density of states obtained by low-T STS [5] and simulated spectra from the FP model for various thickness of Pb films on Ag(111). We will show how the model is sensitive to physical properties of the film like work function or lattice parameter relaxation.

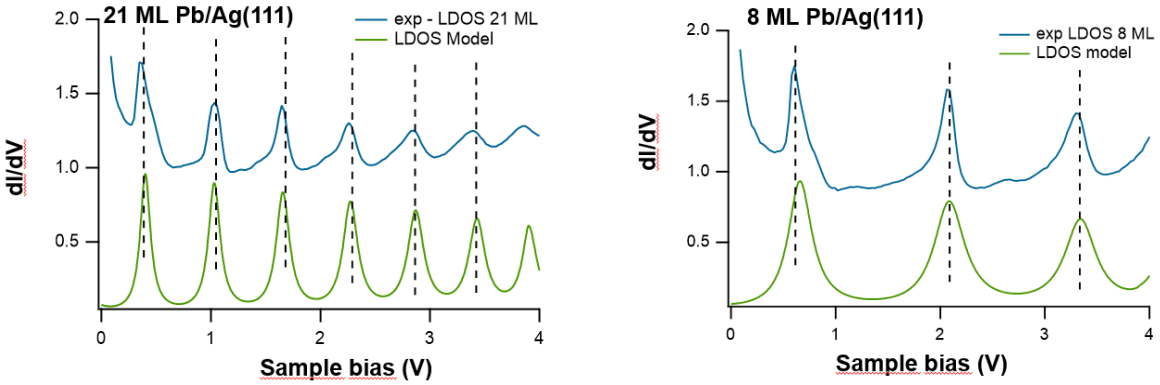

Fig.1. Comparison between the simulated (green) and the measured from STS (blue) local density of states in ultra thin films of Pb epitaxially grown on Ag(111). The simulated spectra are obtained from a Fabry Perot like model adapted to electrons.

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30. Intercalated Transition Metal Dichalcogenide: A structural and electrical study

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Van der Waals materials, composed of crystalline layers bound by weak out-of-plane interactions—such as graphite and transition metal dichalcogenides (TMDs)—provide a versatile platform for property modulation through organic molecule intercalation. Recent studies have demonstrated that intercalating chiral molecules into TaS_2 induces strong current polarization via the *Chirality-Induced Spin Selectivity* (CISS) effect [1]. However, solution-based intercalation methods often suffer from prolonged durations and inhomogeneous results.
A recent breakthrough revealed that galvanic intercalation of thin organic molecules into bulk TMDs achieves near-monolayer behavior [2]. In this work, we present **structural** (Raman spectroscopy, Raman photoluminescence, X-ray diffraction) and **electrical** (current-voltage, *I-V*) evidence of galvanic intercalation of **L-Cysteine methyl ester** into TMDs. Our findings demonstrate controlled and homogeneous modification of material properties, paving the way for applications in spintronics and molecular electronics.

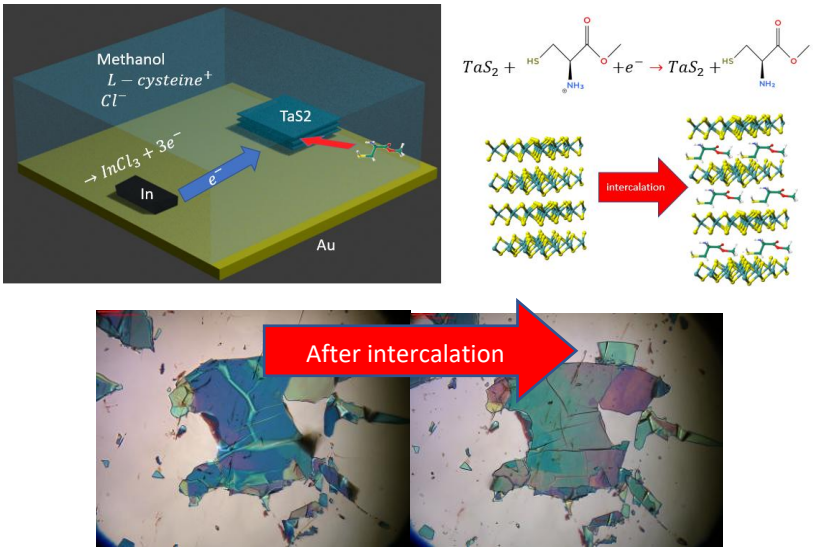

Fig.1: Schematic of the intercalation mechanism (top) and images (bottom) taken with an optical microscope (x100) before and after galvanic intercalation (L-cysteine methyl ester 50mM), *schematics source: molstar, wikipedia*

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31. Elaboration de films minces épitaxiés de $BaTaO_2N$ dédiés à la photoélectrolyse de l'eau pour une production d'hydrogène décarbonées.

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La transition énergétique requiert le développement de matériaux innovants capables d'assurer efficacement la conversion et/ou le stockage des énergies renouvelables. Parmi les approches explorées, la photoélectrolyse de l'eau apparaît comme une voie prometteuse pour la production d'hydrogène vert à partir de l'énergie solaire. Toutefois, ses performances restent limitées par les matériaux actuellement disponibles, soit à cause de la mauvaise absorption du spectre solaire, soit par des recombinaisons de charges trop importantes [1].
Les oxydes sont d'une stabilité chimique remarquable mais n'absorbent qu'une faible partie du spectre visible. L'oxynitrure pérovskite $BaTaO_2N$ apparaît comme un candidat intéressant pour être utilisé comme photoanode, grâce à sa bande interdite réduite qui permet l'absorption d'une large partie du spectre visible, ainsi qu'à sa ferroélectricité favorisant potentiellement la séparation des charges [2]. Néanmoins, la réalisation de couches minces de haute qualité cristalline, condition essentielle pour obtenir de bonnes performances photocatalytiques et ferroélectriques, demeure un défi.
Dans ce travail, nous présentons la croissance de films minces épitaxiés de $BaTaO_2N$ obtenus par épitaxie par jets moléculaire assistée par plasma d'azote atomique (N-MBE) en utilisant des sources de métaux ultrapurs. La cristallinité a été suivie *in situ* par diffraction des électrons (RHEED) et a ensuite été confirmée *ex situ* par diffraction des rayons X. L'influence de l'épaisseur des films, de la nature des substrats et de l'utilisation de couches tampons a été étudiée de manière systématique, en utilisant les substrats pérovskites Nb:$SrTiO_3$ et $SrTiO_3$. Une couche tampon de $BaTiO_3$, partageant l'élément Ba et présentant un paramètre de maille proche de celui du $BaTaO_2N$, a également été évaluée et s'est révélée prometteuse. La composition chimique a été quantifiée par spectroscopie de photoélectrons X.
Cette étude met en évidence la faisabilité de la croissance contrôlée de $BaTaO_2N$ par N-MBE et souligne le rôle déterminant de l'ingénierie des substrats et des interfaces dans la maîtrise des propriétés structurales de cet oxynitrure prometteur. Ces résultats ouvrent la voie à l'optimisation de son activité pour la photoélectrolyse de l'eau.

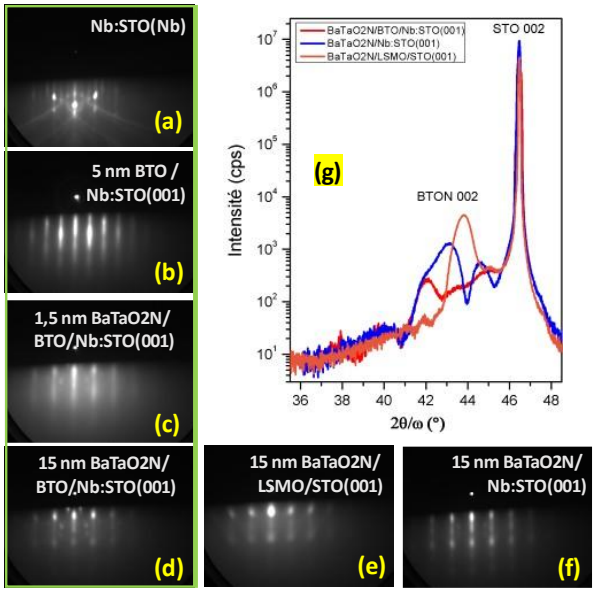

Figure 2. Images RHEED (a) du substrat de Nb:STO(001), (b) de la couche tampon de $BaTiO_3$, (c) du $BaTaO_2N$ au cours de la croissance et (d) (e) (f) en fin de croissance sur différente substrats, et (g) leur courbe de diffraction des rayons X.

Cette recherche a été financée par l'Agence nationale de la recherche au titre du ***projet ANR-24-CE08-1406-01 (FORLIGHT)***

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32. Atomic-Scale Mechanisms of CO Adsorption and O_2 Activation at Au/TiO_2(110) Interfaces: A DFT and In-Situ Perspective

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Understanding how oxygen is activated and how CO adsorbs and reacts at the perimeter between gold nanoparticles and TiO_2 supports is essential for tailoring low-temperature CO oxidation catalysts. Here we present an atomic-scale investigation combining density functional theory (DFT) calculations and insights from recent in-situ transmission electron microscopy to identify preferred adsorption geometries, charge transfer pathways, and active interfacial oxygen species that promote O2 activation at the Au–TiO_2(110) boundary. These observations build on reports of dynamic restructuring of the Au–TiO2 interface under reaction conditions and on size/shape-dependent activity of subnanometer Au clusters. [1][2].

We performed systematic DFT modeling of Aun/TiO_2(110) model systems (n = 6–20) to compute CO and O_2 adsorption energies, characterize O_2 binding modes (molecular, superoxo, peroxo), and map reaction pathways for O_2 dissociation and CO oxidation using CI-NEB. Charge analysis and projected DOS reveal that electron transfer from reduced TiO_2 sites and interfacial Au–O species stabilizes activated O_2 and lowers dissociation barriers, enabling Au-assisted Mars–van-Krevelen or Langmuir–Hinshelwood pathways depending on cluster size and interface oxidation state [3,4]. Our computed energetics and identified transition states are consistent with combined theoretical–experimental mechanistic studies of CO oxidation on Au/TiO_2.

These results clarify how interfacial geometry, support defects, and cluster size conspire to determine the dominant oxidation mechanism and the catalytic turnover at near-ambient conditions. The combined DFT predictions and comparison with in-situ ETEM observations suggest experimental signatures (e.g., O 1s XPS components, CO TPD shifts, and reversible epitaxial rotations of Au) that can be used to validate the proposed mechanisms and to guide rational design of more active and stable Au/TiO_2 catalysts. Our study highlights the importance of controlling interface oxidation and cluster morphology to optimize low-temperature CO oxidation.

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33. Photoelectron diffraction of twisted bilayer graphene

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Twisted bilayer graphene (TBLG) is one of the simplest van der Waals heterostructures, yet it exhibits an exceptionally rich variety of electronic properties that are strongly governed by the twist angle and by the local atomic arrangement within the moiré supercell. While correlated insulating states, superconductivity, circular dichroism, quasicrystalline order, and unconventional pairing mechanisms have been reported at specific twist angles [1-4], experimental access to the underlying structural information remains limited. In this work, we assess the capability of photoelectron diffraction (PED) to probe stacking, twist angle, and local atomic configurations in bilayer graphene [5].

PED measures the angular distribution of core-level photoelectrons, whose intensity results from multiple-scattering and interference effects. Due to the intrinsic complexity of these processes, quantitative interpretation requires comparison with *full multiple-scattering* simulations, which we perform using the MsSpec code [6].

Our calculations demonstrate that PED is highly sensitive to the stacking configuration of bilayer graphene. AA and AB (Bernal) stackings can be unambiguously distinguished through their characteristic sixfold and threefold symmetries, respectively. This contrast originates from interlayer photoelectron scattering, whereby electrons emitted from one layer are diffracted by carbon atoms in the adjacent layer. Layer-resolved PED patterns reveal distinct angular distributions associated with dominant in-plane scattering in the top layer and forward-focusing effects for emitters in the bottom layer. These features provide robust and direct fingerprints of the interlayer stacking geometry in bilayer graphene.

When a twist is introduced between the two layers, the PED response evolves markedly. At high kinetic energies, stacking information is progressively averaged out due to the presence of many inequivalent atomic environments. In this regime, however, PED provides a straightforward and accurate determination of the twist angle through azimuthal scans. At lower kinetic energies, PED becomes sensitive to the atomic arrangement within the moiré supercell.

Our results demonstrate that PED, combined with full multiple-scattering calculations, is a powerful and versatile probe of both global and local structural properties in twisted bilayer graphene. These findings open promising perspectives for experimental investigations of more complex van der Waals heterostructures, multilayer graphene systems, and intercalated structures.

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34. Revolutionising depth profiling XPS with Femto-Second Laser Ablation

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XPS is a very surface sensitive technique, so to investigate changes to the chemistry on the layers below the surface the experiment method involves depth profiling the material by interleaving analysis with removal steps, commonly using ion beams. However, ion beam methods induce changes in the material chemistry, affecting the validity of the results.
Here we are presenting the most recent developments offering the capability of performing depth profiling with a femtosecond laser with a 1030 nm peak wavelength and a pulse duration of 160 fs. Depth profiling has been carried out using traditional monatomic and gas cluster ion beam (GCIB) bombardment and compared to profiles recorded using a new femtosecond laser ablation method.
In the examples shown in this poster, the monatomic and cluster ion sputtering depth profiles exhibited chemical damage due to preferential sputtering of certain atomic species and preferential sputtering artefacts. Femto-seconds depth profiles fully retained the true chemical composition of the large thick layers over hundreds of nanometers and even dizains of microns.

This revolutionary technique has been implemented in our newly developed system Hypulse, the newest member of the ThermoFisher XPS family based on a customized version of the most widely used new generation ThermoFisher XPS system in the field, the Nexsa G2.
This system benefits from the CISA workflow compatibility allowing to perform XPS with Femto-second depth profiling analysis and SEM on the very same region of interest.

Fig.1. Hypulse XPS System (10 micrometer small spot high energy X-Ray source, Femto-Second Laser Ablation)