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ABSTRACT BOOKLET

7th European Workshop on
Epitaxial Graphene & 2D Materials

May 18–21, 2026 · Fredericia, Denmark
Trinity Hotel & Conference

/ Oral & Poster Abstracts

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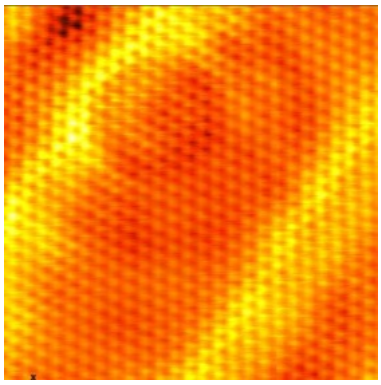
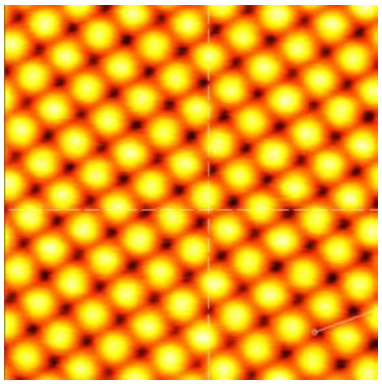


STM: Au(111) @ **3.6 K**



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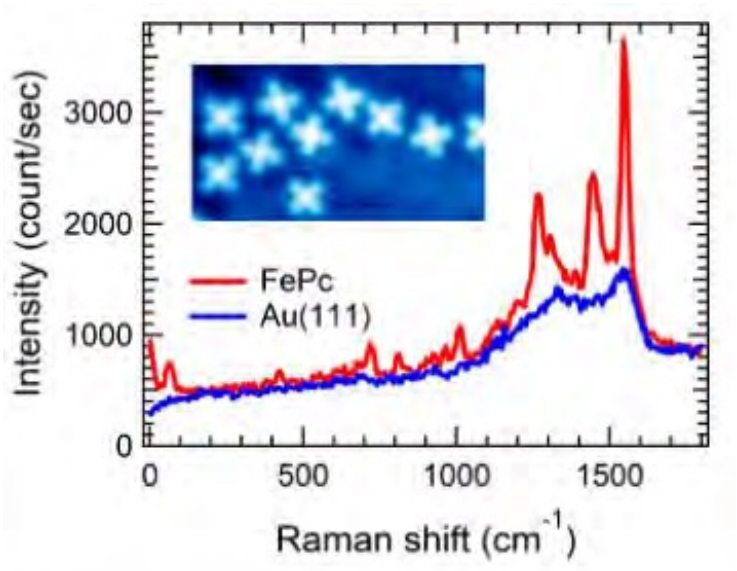

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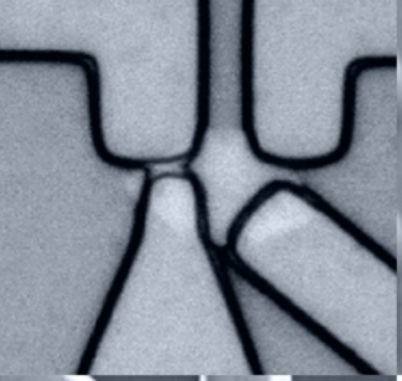
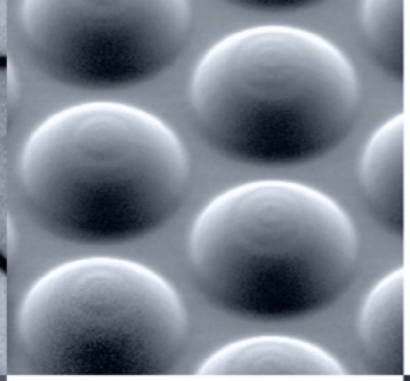

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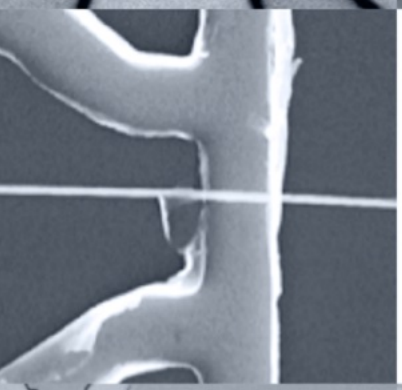

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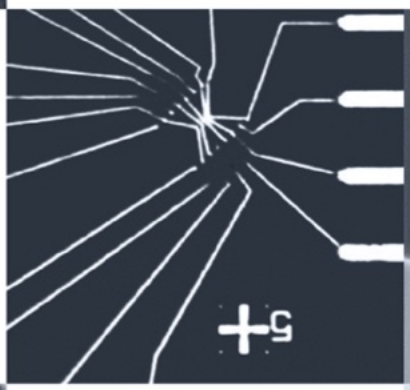
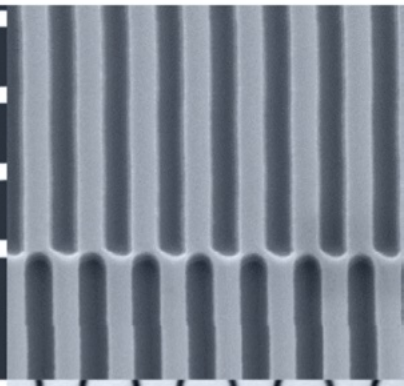
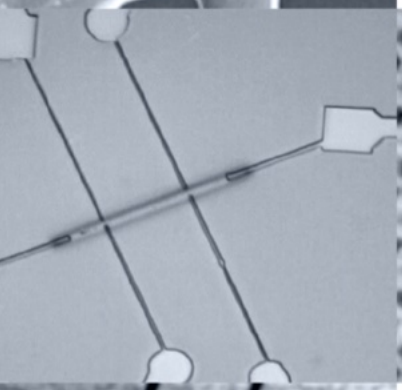
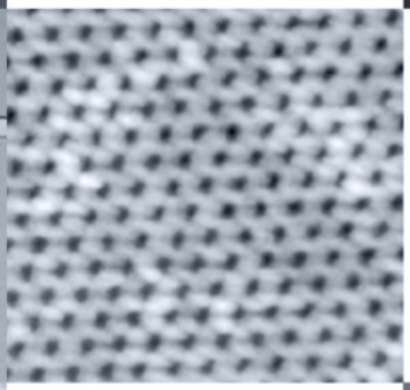

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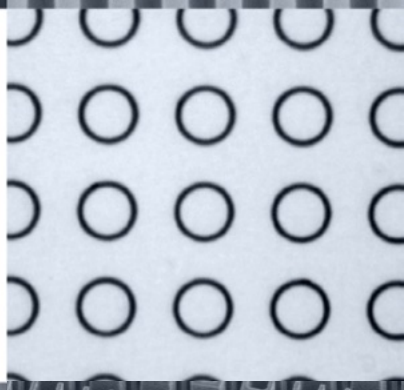
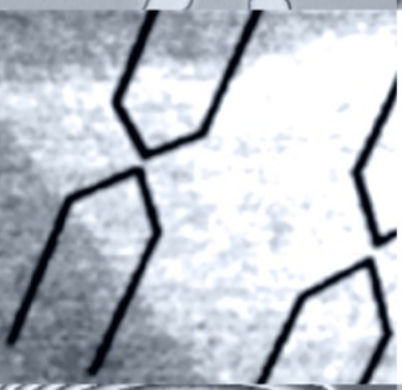

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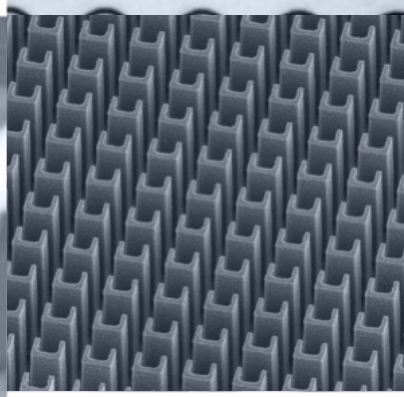

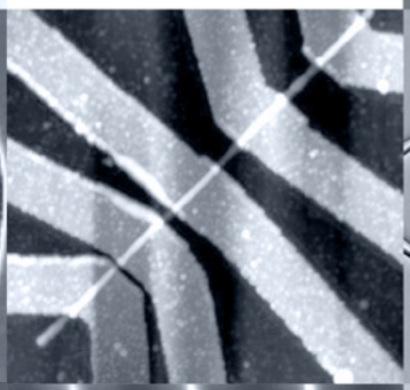
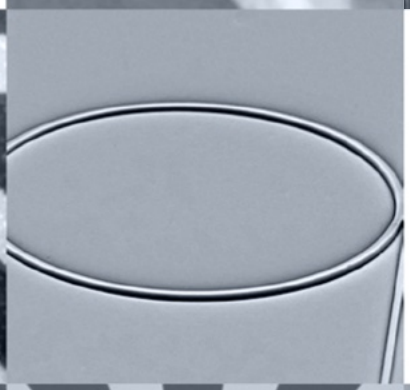

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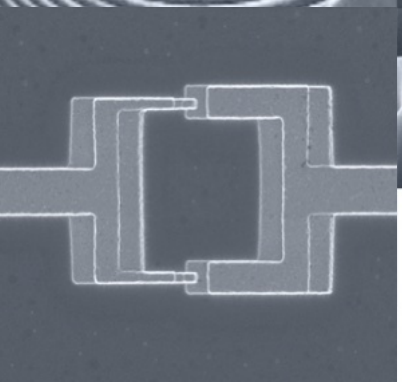
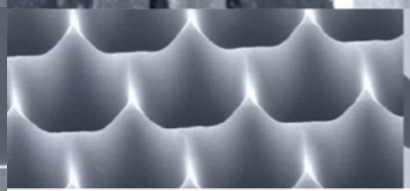

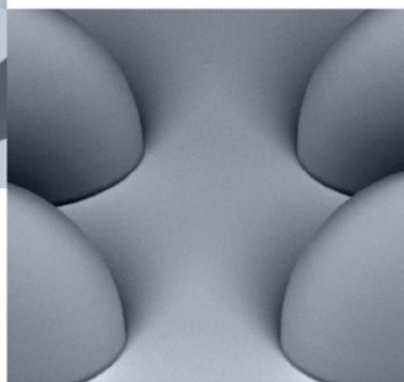

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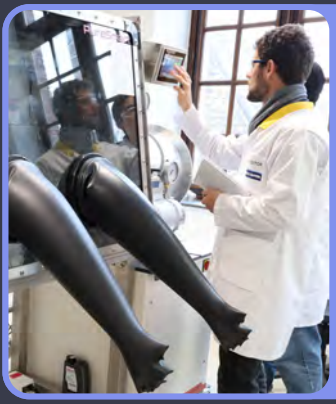

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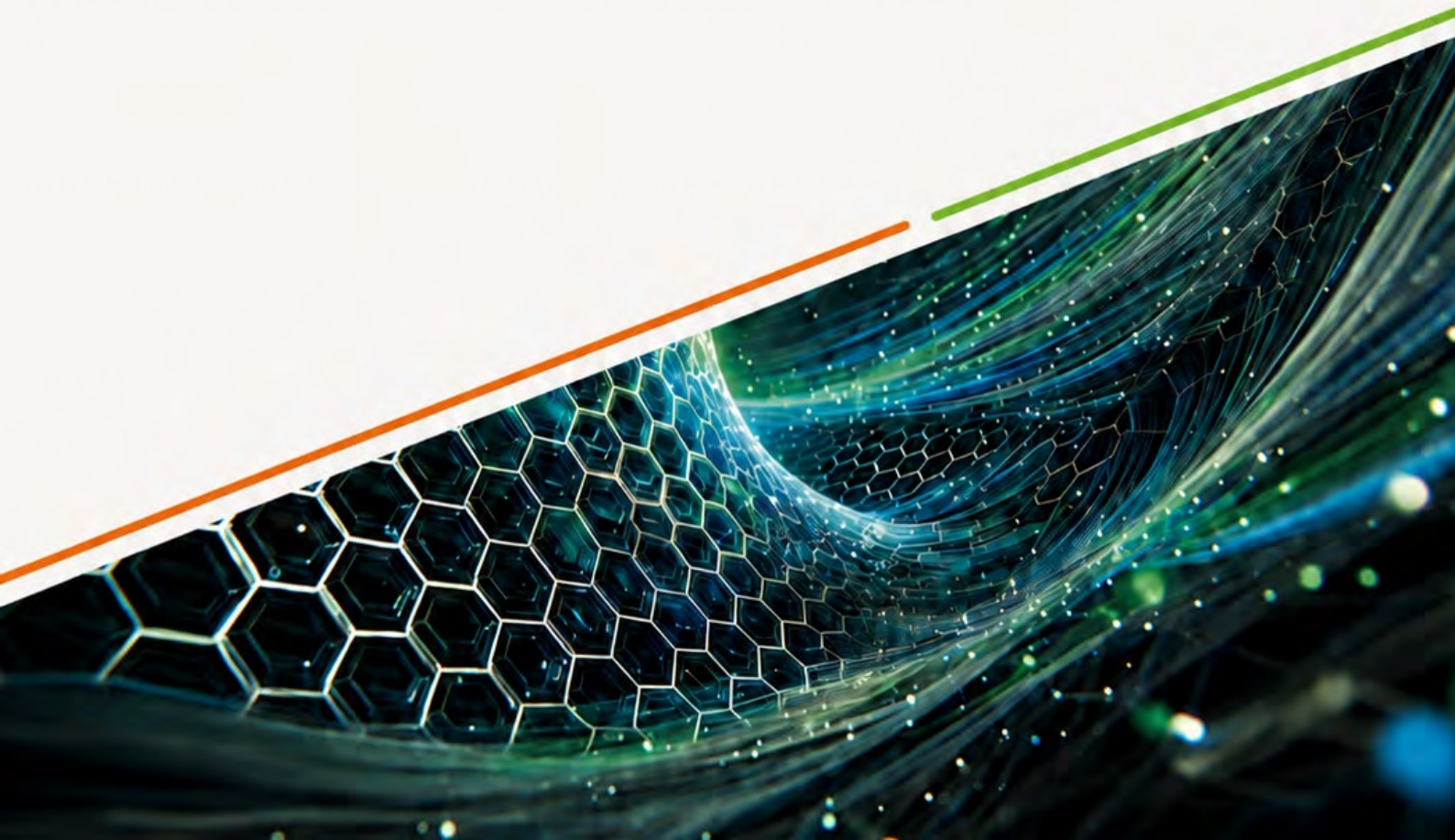
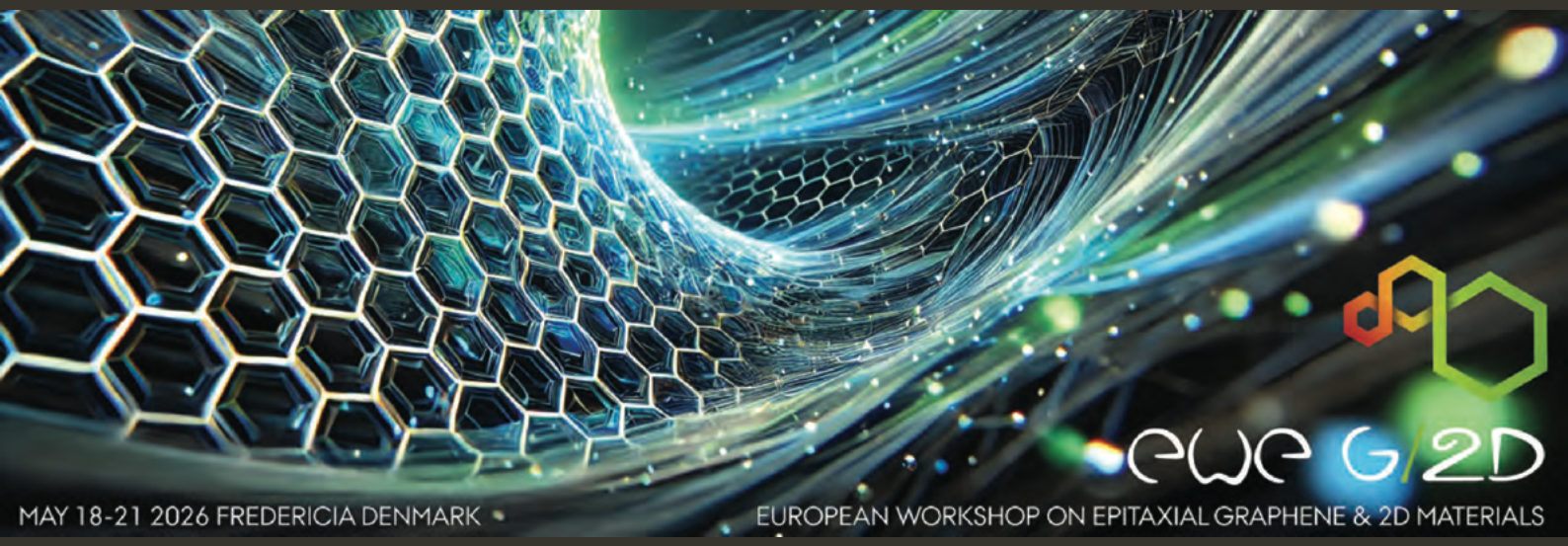
TALK ABSTRACTS





DAY 1

Arrival

14:30 - 15:45	Registration
15:45 - 16:00	Welcome & Opening Remarks

Chair: **Jill Miwa**

16:00 - 16:45	Keynote: **Roman Fasel**- Nanographene-based designer quantum spin systems
16:45 - 17:05	Highlight: **James McHugh** - Spin splitting and band-edge renormalisation in monolayer TMDs
17:05 - 17:25	Highlight: **Stefania Pagliara** - Tracking photoinduced dynamics in layered semi-conductors with ultrafast spectroscopies

19:00 - 20:30	**Dinner**

Nanographene-based Designer Quantum Spin Systems

C. Zhao[1], G. Catarina[1], C.A. Pignedoli[1], J. Ma[2], X. Feng[2], P. Ruffieux[1], J. C. G. Henriques[3], J. Fernández-Rossier[3], R. Fasel[1]

1) Empa – Swiss Federal Laboratories for Materials Science and Technology, nanotech@surfaces Laboratory, Dübendorf, Switzerland

2) Faculty of Chemistry and Food Chemistry, and Center for Advancing Electronics Dresden, Technical University of Dresden, Germany

3) International Iberian Nanotechnology Laboratory, Braga, Portugal

Recent advancements in on-surface synthesis enable the fabrication of unprotected open-shell nanographenes and provide a platform to realize and explore quantum spin models. This presentation addresses three distinct nanographene-based spin chains: (*i*) spin-½ Heisenberg chains formed by covalently linked olympicenes (Fig. 1) [1], (*ii*) spin-1 Haldane chains constructed from triangulenes [2], and (*iii*) spin-½ alternating-exchange Heisenberg chains derived from Clar's goblet molecules [3,4].

We use on-surface synthesis, hydrogenation, and STM tip-induced dehydrogenation [5] to define chain length, parity, and termination with atomic precision. We probe spin excitations by inelastic electron tunneling spectroscopy and support the analysis with high level theoretical calculations. The results follow established quantum spin theory: Integer spin chains show gapped excitations, while half integer spin chains remain gapless. We observe spin fractionalization in spin-1 Haldane chains and spinon excitations in spin-½ Heisenberg chains. For alternating exchange chains, we resolve three distinct phases set by ground state degeneracy and edge excitations. Fourier analysis of inelastic tunneling spectra further yields the dispersion of triplons, which are bosonic spin-1 quasiparticles.

These results demonstrate the capability of bottom-up synthesis combined with STM to construct and probe fundamental quantum spin systems with strong exchange interactions. The approach enables the design of carbon-based quantum materials with tailored spin properties and provides a route to explore their relevance for future quantum technologies.

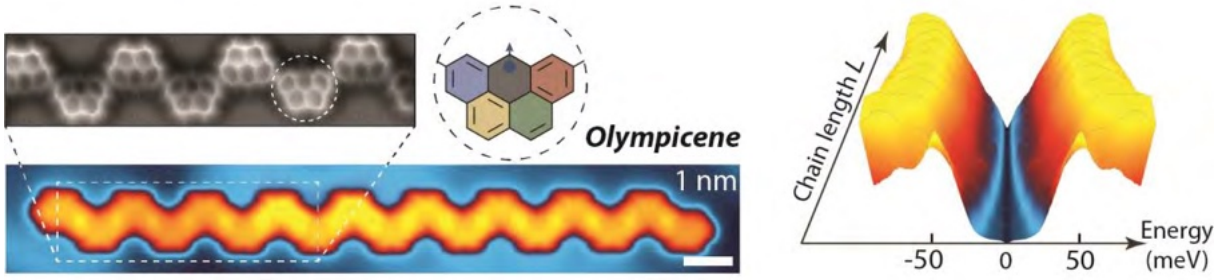


Figure 1: SPM characterization of Heisenberg spin-½ chain (left), and determination of spin excitation gap by inelastic electron tunnelling spectroscopy on chains of increasing length.

References

[1] C. Zhao, L. Yang, J. C. G. Henriques, *et al*., *Nat. Mater*. **24,** 722–727 (2025).
[2] S. Mishra, G. Catarina, F. Wu, *et al*., *Nature* **598**, 287–292 (2021).
[3] C. Zhao, G. Catarina, J.-J. Zhang, *et al*., *Nat. Nanotechnol*. **19**, 1789-1795 (2024).
[4] S. Mishra, D. Beyer, K. Eimre, *et al*., *Nat. Nanotechnol*. **15**, 22–28 (2020).
[5] C. Zhao, Q. Huang, L. Valenta, *et al*., *Phys. Rev. Lett*. **132**, 046201 (2024).

Spin Splitting and Band-Edge Renormalisation in Monolayer TMDs

James G. McHugh[1,2], Igor Rozhansky[1,2], Xue Li[1,2], Suad Alshammari[1,2], Vladimir I. Fal'ko[1,2]

1) Department of Physics and Astronomy, University of Manchester, Oxford Road, Manchester, M13 9PL, United Kingdom

2) National Graphene Institute, University of Manchester, Booth St. E., Manchester, M13 9PL, United Kingdom

In this talk, I will present our recent work showing that the conduction-band spin-orbit (SO) splitting in monolayer MoS_2 is substantially larger than predicted by conventional Density Functional Theory (DFT). Through comparison with magnetotransport measurements, we extract the threshold density for filling the upper spin-split K-point band edge and combine this with many-body theory to show that exchange enhancement explains only part of the observed effect. The remaining discrepancy suggests that standard DFT underestimates the hybridisation of metal and chalcogen orbitals. I will then show how a refined DFT+U+V description, including inter-site Hubbard corrections, yields a much-improved account of conduction-band SO splitting, valence-band splitting, and quasiparticle gap, across the full class of MX_2 TMDs, where M=Mo,W; X =S,Se. These results suggest an efficient and practical route towards more accurate band-edge modelling in 2D semiconductors and further highlight the broader importance of incorporating off-site Hubbard corrections in first-principles descriptions of 2D materials, where weak screening enhances inter-orbital hybridisation and strongly influences the low-energy physics.

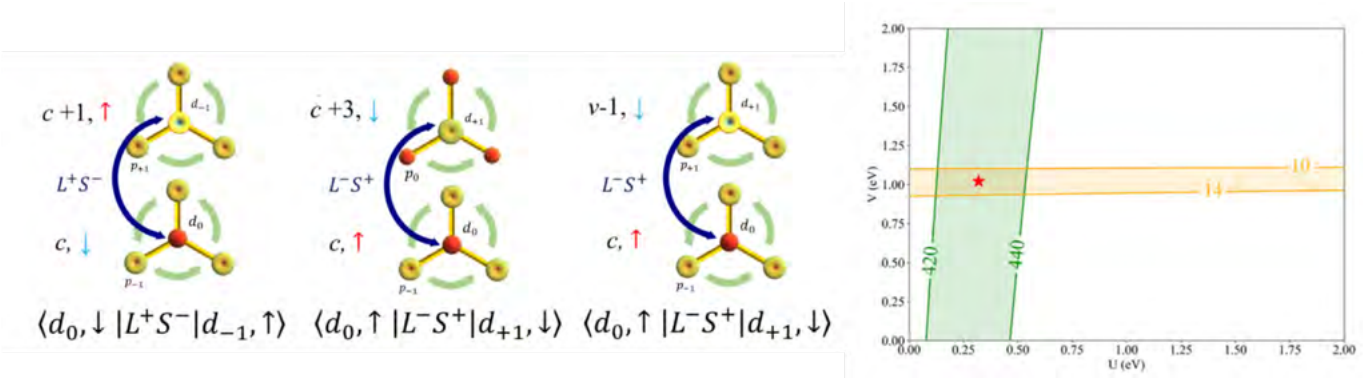


Figure 1: (**Left**) Second-order processes, involving metal (M) and chalcogen (X) orbitals, control the measured conduction band SO splitting in TMDs. (**Right**) By adding Hubbard U+V terms to standard DFT, we can change inter-site hybridisation between M and X species, and correct the spurious underestimation of SO splitting. These tunable parameters bring both the valence (green) and conduction (yellow) band edge SO splitting much closer to experimental values, as compared to "standard" DFT.

References

[1] I. Rozhansky et al., arXiv:2602.09858 (2026).
[2] X. Li et al., Long-range Coulomb Interactions and Spin-Splitting in Transition Metal Dichalcogenides.
[3] K. Marinov et al., Nat. Commun. 8, 1938 (2017).
[4] R. Pisoni et al., Phys. Rev. Lett. 121, 247701 (2018).
[5] C. Robert et al., Nat. Commun. 11, 4037 (2020).
[6] I. Rozhansky and V. Fal'ko, Phys. Rev. B 110, L161404 (2024).

Tracking photoinduced dynamics in layered semiconductors with ultrafast spectroscopies

Stefania Pagliara,[1]

1) *Interdisciplinary Laboratories for Advanced Materials Physics (I-LAM) and Department of Mathematics and Physics, Università Cattolica, I-25133 Brescia, Italy*

e-mail presenting author: stefania.pagliara@unicatt.it

Ultrafast photoexcitation of layered semiconductors leads to the formation of stable excitonic features, making these systems an ideal platform for investigating excitonic many-body interactions and their coupling to lattice and spin degrees of freedom on ultrafast timescales. The goal of this talk is to present experimental protocols based on ultrafast optical and photoemission spectroscopies that enable direct access to excitonic resonances and allow the investigation of their fundamental many-body interactions.

At low temperatures and under quasi-resonant excitation conditions, coherent light–matter interactions can transiently generate a coherent excitonic state, which typically persists for only a few femtoseconds, making its experimental observation particularly challenging. Since quantum coherence is a key ingredient for next-generation technologies, this limitation can be overcome by carefully selecting the layered material and optimizing the experimental parameters in transient optical spectroscopy measurements [1]. Following the coherent-to-incoherent exciton crossover, exciton dynamics evolve on timescales ranging from femtoseconds to several picoseconds, governed by exciton–exciton interactions and coupling to other quasiparticles such as quasi-free carriers and phonons. Time-resolved broadband optical spectroscopy provides direct access to exciton–phonon coupling by identifying spectral fingerprints of the optical response and demonstrating that excitonic resonances can be optically modulated through coupling to coherent atomic vibrations, whose spatial extent can be estimated with sub-picometer resolution [2,3]. In addition, time- and angle-resolved photoemission spectroscopy enables the investigation of exciton formation and subsequent relaxation dynamics in the time, energy, and momentum domains [4].

Extending this framework to layered magnetic semiconductors, polarized and time-resolved broadband optical spectroscopy reveals clear signatures of the coupling between selected optical phonons and the underlying magnetization. These results demonstrate polarization-dependent phonon generation and highlight the interplay among lattice, magnetic, and electronic degrees of freedom.

References

[1] V. Gosetti, J. Cervantes-Villanueva, D. Sangalli, A. Molina-Sánchez, V. F. Agekyan, C. Giannetti, L. Sangaletti, S. Mor, S. Pagliara, "*Detection of a coherent excitonic state in the layered semiconductor BiI_3*", *ACS Photonics* ***11****, 2513-2520 (2024)*

[2] S. Mor, V. Gosetti, A. Molina-Sánchez, D. Sangalli, S. Achilli, V. F. Agekyan, P. Franceschini, C. Giannetti, L. Sangaletti, S. Pagliara "*Photoinduced modulation of the excitonic resonance via coupling with coherent phonons in a layered semiconductor*", Phys. Rev. Research **3**, 043175 (2021)

[3] S. Mor, V. Gosetti, V. F. Agekyan, C. Giannetti, L. Sangaletti, S. Pagliara, "*Effect of photoinduced screening on the spectroscopic signature of exciton-phonon coupling*" *ACS Photonics* ***11****, 2282-2288 (2024)*

[4] V. Gosetti, J. Cervantes-Villanueva, S. Mor, D. Sangalli, A. García-Cristóbal, A. Molina-Sánchez, V. F Agekyan, M. Tuniz, D. Puntel, W. Bronsch, F. Cilento, S. Pagliara, "*Unveiling the exciton formation in time, energy and momentum domain in layered van der Waals semiconductors*", Progress in Surface Science 100, 100777, (2025)

DAY 2

7:00 - 9:00	**Breakfast**
	Chair: **Carsten Busse**
9:00 - 9:30	Invited: **Kristian Sommer Thygesen** - Building a digital infrastructure for 2D materials science
9:30 - 10:00	Invited: **Justin Wells** - Further enchancing the usually strong electron-phonon kinks in graphene and hBN
10:00 - 10:20	Contributed: **Miguel A. Valbuena** - Engineering a spin-orbit bandgap in graphene-tellurium-irridium heterostructures
10:20 - 10:40	Highlight: **Alberto Turoldo** - Interfacial oxidation enables charge-transfer contacts and degenerate n-doping in monolayer MoS2
10:40 - 11:10	**Coffee**
	Chair: **Carsten Busse**
11:10 - 11:40	Invited: **Antonija Grubišić-Čabo** - Preparation of large-area 2D materials using UHV-based KISS method
11:40 - 12:00	Contributed: **Catherine Grover** - Epitaxial growth of pristine 2D Ta-S-Se Janus membranes on Au(111)
12:00 - 12:20	Contributed: **Abdallah Karaka** - Co2S2: a new 2D material and its phase transitions
12:20 - 12:40	Contributed: **Matthias Batzill** - Mirror twin boundary phases in MoTe2
12:40 - 14:10	**Lunch**
	Chair: **Thomas Michely**
14:10 - 14:40	Invited: **Niklas Witt** - Dirac meets flat band: real-space switching of local moments driven by quantum geometry in correlated graphene heterosturctures
14:40 - 15:00	Contributed: **Guangyao Miao** - Doping monolayer graphene to the Van Hove singularity
15:00 - 15:20	Contributed: **Affan Safeer** - Small polarons in single layer MnBr2: substrate dependence and interaction with a super-moiré
15:20 - 15:40	Contributed: **Anshika Mishra** - Manipulation of polarons in monolayer NiBr2
15:40 - 16:10	**Coffee**
	Chair: **Thomas Michely**
16:10 - 16:40	Invited: **Peter Liljeroth** - Mangetic excitations in van der Waals quantum materials at the atomic scale
16:40 - 17:00	Contributed: **Dominik Legut** - Perpendicular mangetic anistropy in a single Dy adatom ferrimagnet
17:00 - 17:20	Contributed: **Daniel Jansen** - Atomic manipulation on epitaxial 2D materials
17:20 - 17:40	Contributed: **Sandra Sajan** - Atomic-scale mapping of superconducitvity in the incoherent CDW mosaic phase of a transition metal dichalcogenide
19:00 - 20:30	**Dinner**
20:30 - 22:00	Poster Session

Building a Digital Infrastructure for 2D Materials Science

Kristian Sommer Thygesen[1]

1) Technical University of Denmark

Two-dimensional (2D) materials exhibit a rich spectrum of physical properties deriving from their atomic thinness and highly anisotropic bonding pattern. In practice, however, their behavior depends critically on factors such as interlayer coupling, crystal defects, and synthesis-dependent structure and morphology. Revealing, understanding, and addressing this complexity calls for open and integrated resources going beyond the "ideal crystal" paradigm and connecting experiments and theory. 2DHub [1] is an open web platform providing unified access to a number of highly curated and internally consistent databases spanning key aspects of 2D materials. Its backbone, C2DB, contains computed properties for more than 17,000 pristine monolayer crystals. BiDB contains crystal structures and basic electronic properties of around ~3000 homobilayers in all possible lattice matched configurations. HetDB holds the crystal structures and electronic band structures of ~2500 heterobilayers assembled from 100 different monolayers in various low-strain (<0.5%) configurations. QPOD provides access to thermodynamic, electronic, magnetic, and optical properties of more than 14,000 point defect systems, including both single and double defects in more than 50 different 2D host materials. Finally, X2DB is a new database of experimentally realized 2D materials with information about crystal structure, sample morphology, synthesis routes, substrates, and characterization methods. The X2DB is interlinked with the computational databases and supports community uploads. In this talk, I will introduce 2DHub and illustrate how the platform enables a holistic approach to 2D materials research. By unifying and integrating diverse datasets in an accessible infrastructure, 2DHub supports accelerated discovery, reproducibility, and collaboration across the global 2D materials community.

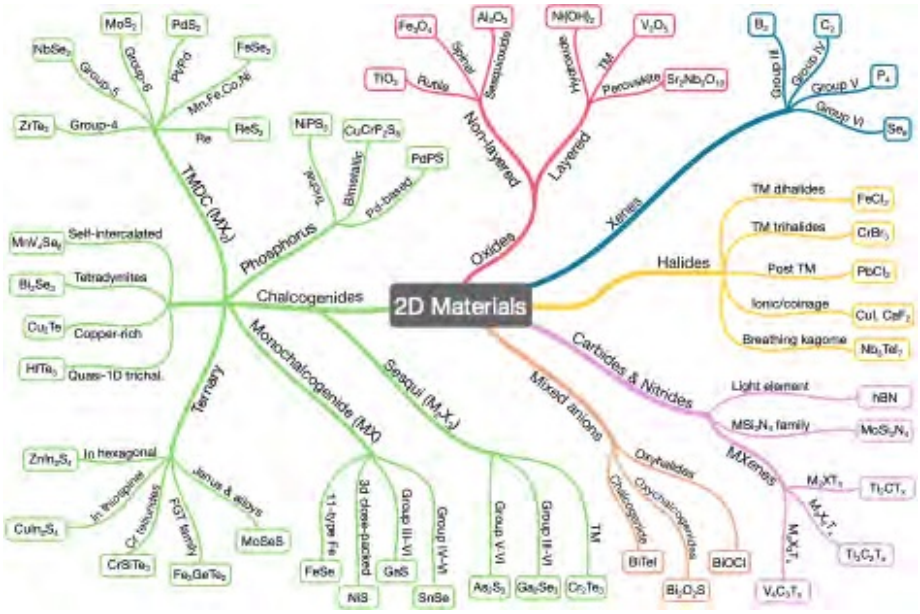


Figure 1: Hierachical classification tree of experimentally realized 2D materials from the X2DB database

References

[1] 2dhub.org

Further enhancing the unusually strong electron-phonon kinks in graphene and hBN

Wells, Justin W.[1]

1) Centre for Materials Science and Nanotechnology and Department of Physics, University of Oslo, Norway

Background: In 2013, we reported strong electron-phonon coupling (EPC) in the σ-bands of graphene [1]. This observation was highly controversial at the time, and attempts were made to dismiss it as a consequence of photoemission matrix elements instead [2]. We endeavoured to clear up this controversy by i) theoretical support and ii) manipulating the photoemission matrix elements by measuring in the neighbouring BZs and on bilayer samples, confirming mass enhancements of $\lambda \approx 0.7$ [3].

Since then, we have predicted that hBN should host similarly strong EPC in its σ-bands [4]. This is unsurprising since the electronic structure, phonon structure, geometry, are all similar to graphene. On the other hand, experimental confirmation adds further credence to our understanding of EPC in graphene's σ-bands. Contrastingly, we predict strong EPC in the π-band of hBN. hBN's π-band has a parabolic maxima, making the EPC arguments (especially the scattering k-space) very different to graphene, and leading to much stronger EPC.

Most recently, we have confirmed the presence of strong EPC in both the π- and σ-bands of hBN. Furthermore, we show that the EPC strength in the π-band depends strongly on doping and/or substrate interaction, thus making it possible to further enhance the EPC (specifically with K and Cl intercalants). Several questions remain unanswered, and are the focus of ongoing work: including further ARPES studies, DFT and helium scattering studies.

In this talk, I will give a short overview of the unusual EPC in graphene's σ-bands, as well as presenting our most recent studies of monolayer hBN with dopants and intercalants. I will briefly present the helium scatting work and conclude with our latest understanding and some as yet unanswered questions.

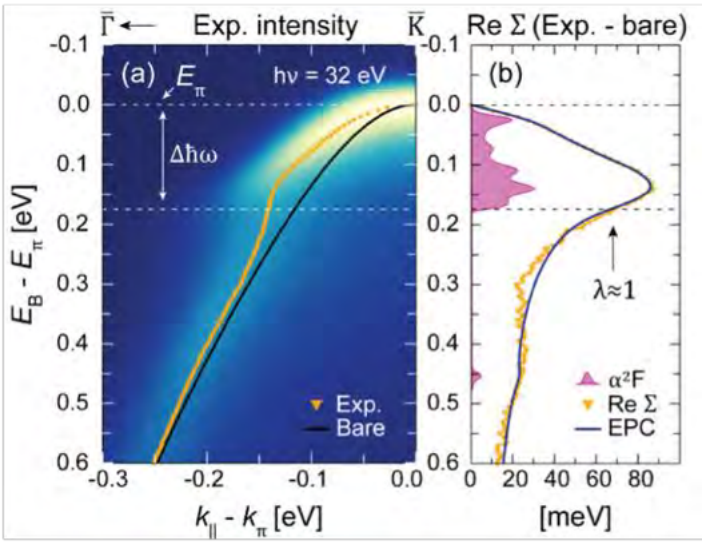


Figure 1: EPC in monolayer hBN. a: Renormalized π-band of monolayer hBN near the high-symmetry K point. b: Experimental self-energy (Re Σ) of the renormalized π-band in a. A large electron mass-enhancement (λ≈1) can be observed Δħω = 175 meV of the band maximum.

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Engineering a spin-orbit bandgap in graphene-tellurium-iridium heterostructures

B. Muñiz Cano[1], F. Calleja[1], D. Pacilè[2], M. G. Cuxart[1], M. Pisarra[2], A. Sindona[2], F. Martín[3], E. Salagre[3], P. Segovia[3], E. G. Michel[3], A. L. Vázquez de Parga[3], R. Miranda[1,3], J. Camarero[1,3], Manuela Garnica[1], and **Miguel A. Valbuena[1]**

1) IMDEA Nanociencia, Madrid, Spain.
2) Università della Calabria, Italy.
3) Universidad Autónoma de Mddrid, Spain.

Engineering a sizable bandgap and tailoring spin–orbit coupling (SOC) in graphene are key steps toward its implementation in next-generation electronic and spintronic devices. Among the different proximity routes explored so far, heavy p-block elements remain comparatively underinvestigated. Here, we report on the controlled intercalation of tellurium at the graphene/Ir(111) interface and its impact on the electronic and spin properties of graphene [1].

Low-energy electron diffraction (LEED) and scanning tunneling microscopy (STM) reveal the formation of two distinct intercalated phases, depending on the Te coverage. Angle-resolved photoemission spectroscopy (ARPES) demonstrates the opening of a large bandgap of about 240 meV at the Dirac point, while preserving the characteristic linear dispersion of graphene bands at room temperature. The intercalated system exhibits strong electron doping, in agreement with quasiparticle interference measurements. Reducing the Te coverage allows tuning the Dirac point towards the Fermi level, with the gap remaining robust. Spin-resolved photoemission (SR-ARPES) measurements uncover a complex chiral spin texture with sizable in-plane and out-of-plane spin polarization components. In addition, scanning tunneling spectroscopy reveals signatures consistent with the emergence of an edge state. These findings indicate a substantial enhancement of intrinsic SOC in graphene induced by Te intercalation, going beyond a purely Rashba-type interaction. The graphene/Te/Ir(111) system thus emerges as a versatile platform for investigating spin-dependent transport phenomena and proximity-induced topological phases, including the quantum spin Hall effect.

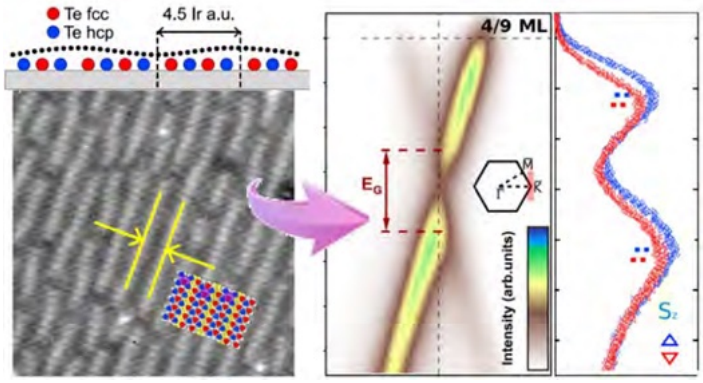

Figure 1: (From left to right). Atomic scale STM image, ARPES graphene Dirac cone and SR-ARPES spin splitting of Gr/Te/Ir(111) heterostructures

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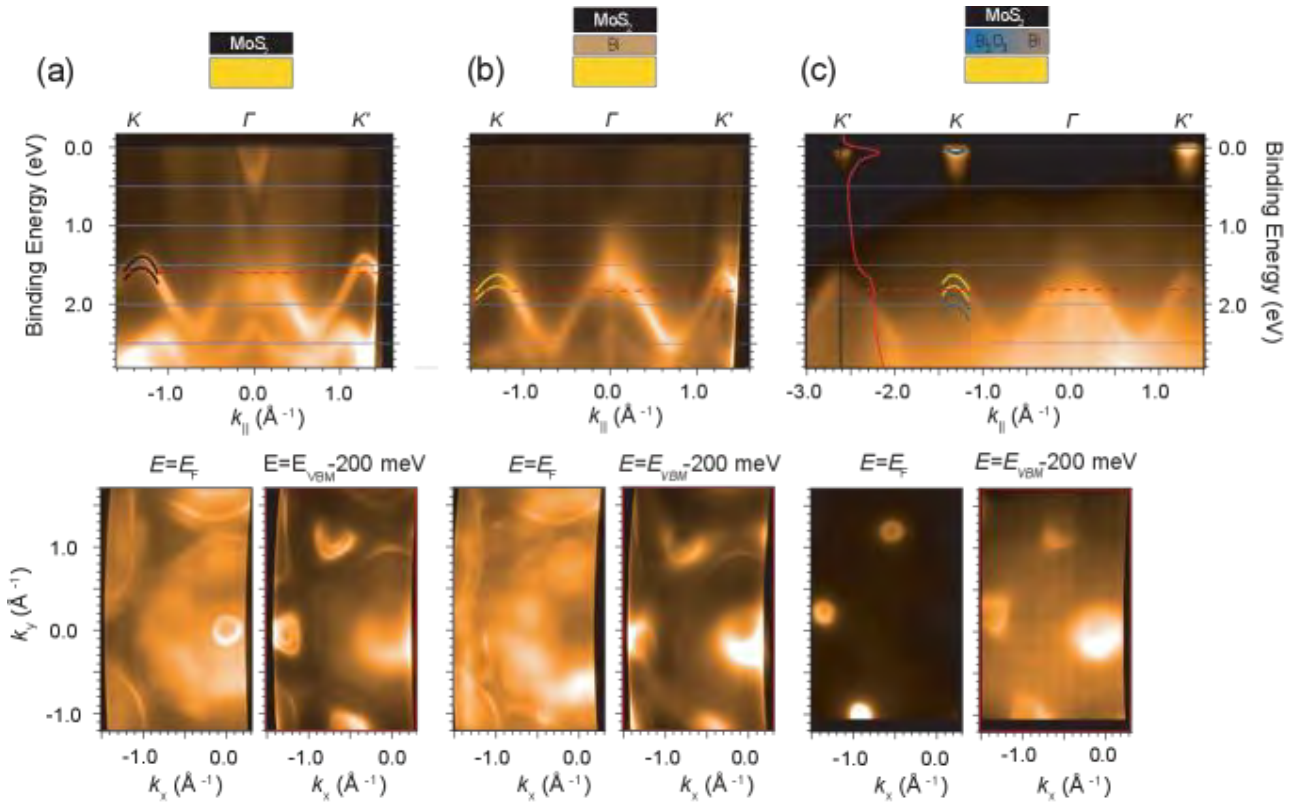
Interfacial Oxidation Enables Charge-Transfer Contacts and Degenerate n-Doping in Monolayer MoS_2

Alberto Turoldo
University of Trieste & Elettra-Sincrotrone Trieste S.C.p.A

High contact resistance remains a central obstacle to the integration of two-dimensional (2D) semiconductors in electronic devices. Recent advances have demonstrated that contact performance can be dramatically improved through interface engineering, including the use of group-V semimetals and charge-transfer contacts based on strong interfacial doping. We show that controlled interfacial oxidation provides an effective route to convert a semimetal contact into a charge-transfer contact that degenerately n-dopes single layer MoS_2. Using a combination of angle-resolved photoemission spectroscopy, X-ray photoelectron diffraction, low-energy electron diffraction and scanning tunnelling spectroscopy, we demonstrate that putting single layer MoS_2 in contact with a pristine Bi layer merely results in weak doping, whereas oxidation of the Bi layer leads to a pronounced occupation of the MoS_2 conduction band with an electron density on the order of 10^{13} cm^{-2}. The cause of this strong electron doping is the fact that an ultrathin β-Bi_2O_3 layer forms below the MoS_2 and that this has a particularly low work function, thereby acting as an efficient electron donor to MoS_2. Interfacial oxidation thus emerges as a powerful design knob for engineering charge-transfer contacts to 2D semiconductors.



Preparation of large-area 2D materials using UHV-based KISS method

Antonija Grubišić-Čabo[1]

1) Zernike Institute for Advanced Materials,

Two-dimensional (2D) materials offer a rich platform for investigating novel quantum phenomena and designing nanostructures with tailored functionalities. However, key characterization techniques such as photoemission spectroscopy impose strict requirements on sample quality, size, and surface cleanliness conditions that are often difficult to meet using standard mechanical exfoliation methods, even within a glove box environment. In this talk, I will present a method for in situ exfoliation of 2D materials, the kinetic *in situ* single-layer synthesis (KISS) method, performed directly under ultra-high vacuum (UHV) conditions [1,2]. This technique enables the preparation of large-area, high-quality flakes with excellent crystallinity, and is particularly well-suited for air- sensitive materials, as it completely avoids exposure to ambient conditions. Using the KISS method, we successfully exfoliated various semiconducting and metallic transition metal dichalcogenides, as well as kagome materials, onto Au, Ag, and Ge substrates, demonstrating the method's broad applicability. The electronic structure of these materials was subsequently probed using angle-resolved photoemission spectroscopy (ARPES), confirming the high quality of the KISS exfoliated samples.

The KISS method is simple, robust, and requires no specialized equipment, making it an accessible and powerful approach for preparing clean, high-quality 2D materials suitable for advanced spectroscopic studies.

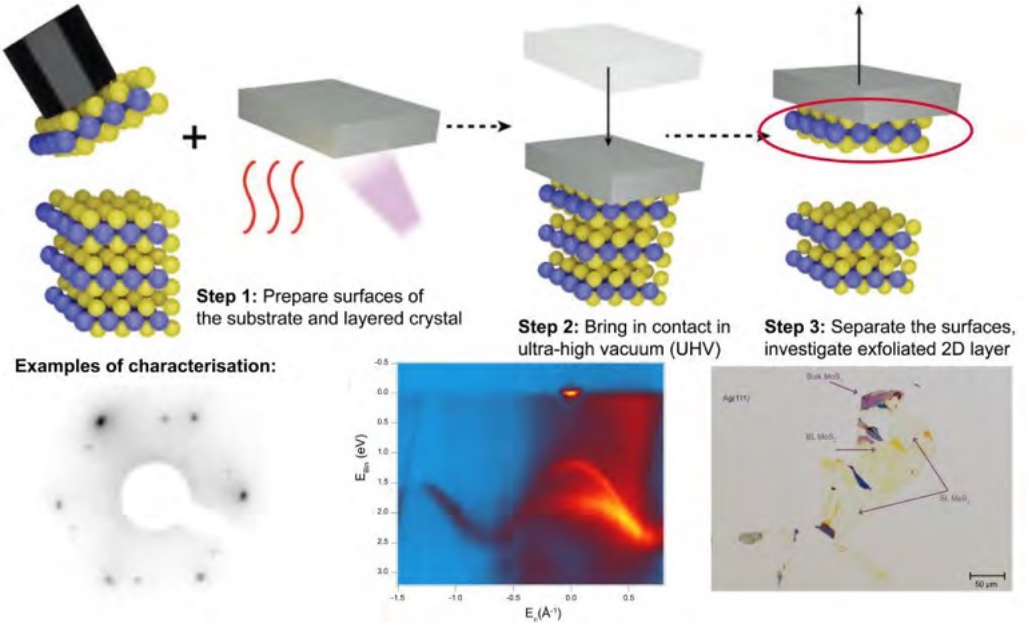


Figure 1: Sketch of KISS exfoliation (top) and examples of characterisation methods, including ARPES (bottom).

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Epitaxial growth of pristine 2D Ta-S-Se Janus membranes on Au(111)

Catherine Grover[1], Alice Bremerich[1], Dina Wilks[1], Carsten Busse[1], and Thais Chagas[1]
1) Department Physik, Universität Siegen, 57072 Siegen, Germany

We report the controlled synthesis and atomic-scale characterization of two-dimensional Ta–S–Se Janus membranes on Au(111) prepared under ultra-high vacuum. . Ta is first deposited onto clean Au(111), followed by annealing in an H_2S atmosphere. Under sulfur-poor conditions, this leads to a tantalum monosulfide (TaS) (Fig. 1 a) [1, 2] that can be converted to the common TaS_2 by further sulfurization [2]. Here, we exploit this layer-wise growth by changing to selenization in the second step. tion. Scanning tunneling microscopy reveals the formation of large-area, well-defined Ta–S–Se islands with atomic precision. These results provide compelling evidence that the islands correspond to Ta–S–Se Janus membranes, establishing a reliable route toward the fabrication of Janus transition-metal chalcogenides with broken out-of-plane symmetry.
We find a similar behaviour in the Ta-Se system, where we can go from TaSe to $TaSe_2$. In consequence, we propose that our growth protocol also allows for the preparation of Janus membranes with inverted polarity.
Our approach enables a higher degree of tunability than previously reported preparation methods, which typically rely on sulfurization of transition-metal diselenides or on the removal of topmost layers via plasmonic H_2 treatment [3].

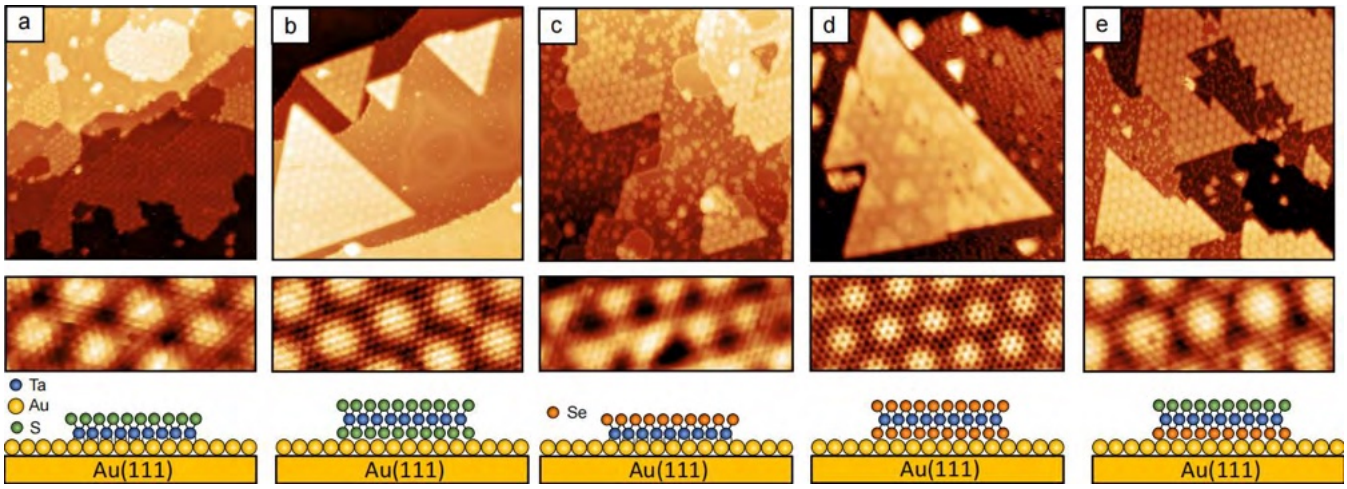

Figure 1: STM images of (top) large-scale islands, (middle) their atomic and moire resolution at a size 14.5 nm x 6.5 nm (bottom) corresponding model for (a) TaS, (b) TaS_2, (c) TaSe, (d) $TaSe_2$ and (e) STaSe. Image Parameters: (a) (top) V = -2.25 V, I = 0.01 nA, (middle) V = -0.91 V, I = 0.10 nA, (b) (top) V = -0.83 V, I = 0.09 nA, (middle) V = -0.44 V, I = 3.80 nA, (c) (top) V = -1.66 V, I = 0.02 nA, (middle) V = -0.14 V, I = 0.14 nA, (d) (top) V = -0.35 V, I = 0.04 nA, (middle) V = -0.35 V, I = 0.58 nA, and (e) (top) V = -1.42 V, I = 0.17 nA, (middle) V = -0.30 V, I = 1.7 nA. Image Sizes: (a) (top) 21.5 nm × 21.5 nm, (b) (top) 46.5 nm × 46.5 nm, (c) (top) 43.5 nm × 43.5 nm, (d) (top) 22.5 nm × 22.5 nm and (e) (top) 49.0 nm × 49.0 nm.

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Co_2S_2: a new 2D material and its phase transitions

Abdallah Karaka,[1] Max Wolfertz,[1] Affan Safeer,[1] Miao Guangyao,[1] Wouter Jolie,[1] Thomas Michely ,[1] and Jeison Fischer,[1]

1) II. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, 50937 Cologne, Germany

Using molecular beam epitaxy under ultra-high vacuum conditions and under conditions far from equilibrium 2D materials can be synthesized for which no bulk parent compound exists.

Co_2S_2-2D is such an example. Using scanning tunneling microscopy, scanning tunneling spectroscopy and low energy electron diffraction we characterize this new single-layer 2D material crystallizing in the CuI structure (space group: P$\bar{3}$m1 trigonal), when grown on graphene on Ir(111) using molecular beam epitaxy. We found it can be synthesized phase pure upon low temperature growth and moderate annealing. Its lattice constant is 3.62 ± 0.01 Å and its height is 6.2 Å. Beyond the single-layer limit it transforms into a new hexagonal crystal structure with a distinctly different lattice parameter of 3.51 ± 0.01 Å, a height of 11.7 Å and a very different dI/dV spectra. This transition typically occurs between 650 and 750 K, although the exact temperature depends on the annealing conditions. The phase transition is accompanied by the emergence of a 2x2 superstructure in the high temperature phase. When the sample is annealed to 900 K, a square crystal structure starts to form with a lattice parameter of 3.50 ± 0.01 Å and a minimum height of 2.38 nm.

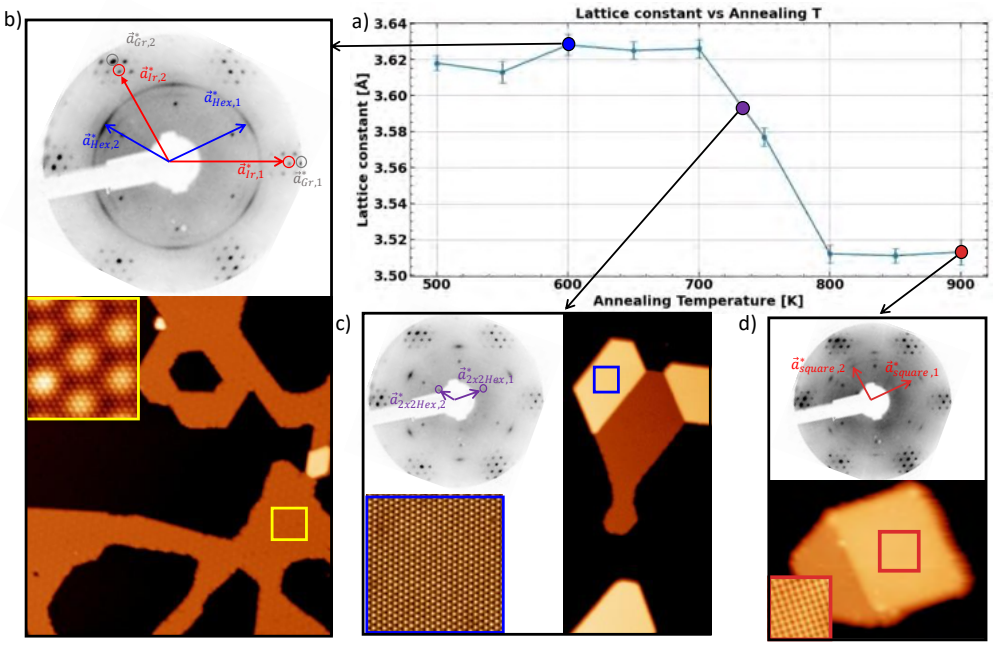

Figure 1: Annealing sequence and phase changes of Co_2S_2 : (a) Lattice parameter as a function of annealing temperature. (b) Contrast-inverted 100 eV LEED pattern and STM overview image of Co_2S_2 on Gr/Ir(111) after the sample is annealed to 600 K, with the inset in the STM overview showing an atomically resolved STM image of the hexagonal Co_2S_2. (c) Contrast-inverted 100 eV LEED pattern, STM overview and atomically resolved STM images of hexagonal multilayer Co_xS_y exhibiting a (2x2) superstructure after the sample is annealed to 733 K. (d) Contrast-inverted 100 eV LEED pattern and STM overview image of square Co_xS_y on Gr/Ir(111) after the sample is annealed to 900 K, with the inset in the STM overview showing an atomically resolved STM image of the square Co_xS_y.

Mirror Twin Boundary Phases in $MoTe_2$

Onyedikachi Alanwoko,[1] Daniil Kruklinskii,[2] Mahdi Ghorbani-Asl,[2] Arkady V. Krasheninnikov,[2] and Matthias Batzill[1]

1) Department of Physics, University of South Florida, Tampa, FL 33620, USA
2) Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, 01328 Dresden, Germany

Mirror twin boundaries (MTBs) in 2D transition metal dichalcogenides are chalcogen deficient line defects. Their low formation energy in $MoTe_2$ means that Te-deficiencies can condense into triangular MTB loops (Fig. 1 (a)). We have shown that under optimized conditions (annealing under Te-flux) these triangular MTB loops can form ordered networks with different network periodicities (Fig. 1 (b)) corresponding to slight variations in the materials composition.[1] While there are many possible arrangements of the triangular loops (Fig. 1(c)), only one motif is experimentally observed, with different compositions only changing the length of the triangular loops. Computing a compositional phase diagram of formation energies vs. composition reveals that the observed structures lie on a 'modified' convex hull (Fig. 1(d)), where the reference point for pure Mo is that of Mo-clusters rather than bulk Mo. This indicates that the observed structures are thermodynamic equilibrium phases for nanomaterials in the Mo-Te phase diagram.

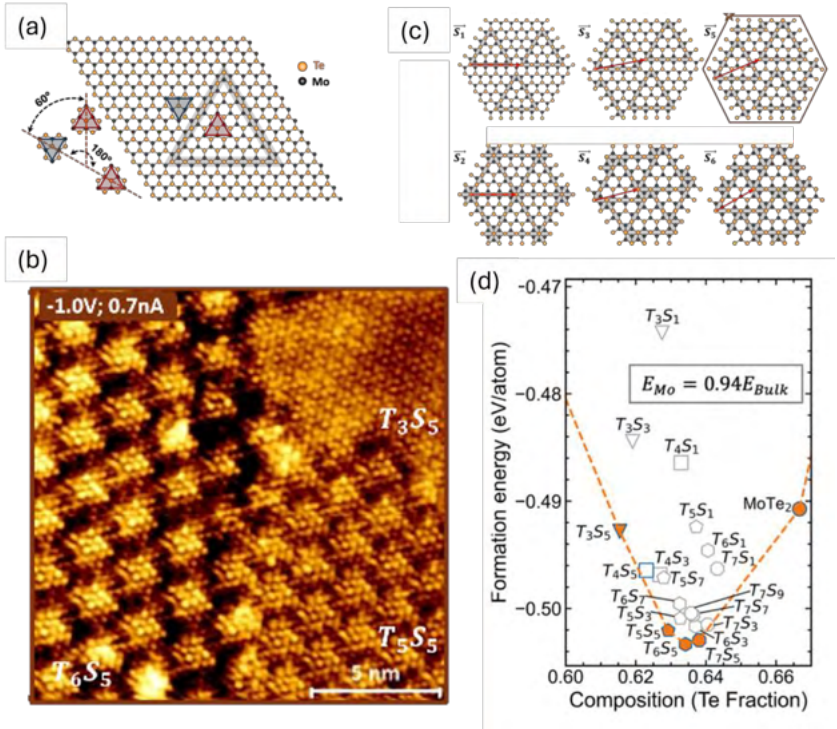

Figure 1: MTB phases in MoTe2. (a) illustration of a triangular MTB loop with MTB indicated by the gray shaded area. (b) STM image of three domains of MTB-phases with different lengths of the triangular loops. (c) possible ordered arrangements of MTB loops, with varying offset vector (indicated by the red arrows) of the triangular loops. (d) computed compositional phase diagram with the formation energies of the possible MTB-phases indicated, The experimentally observed phases are indicated in orange and form the convex hull.

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Dirac meets flat band: Real-space switching of local moments driven by quantum geometry in correlated graphene heterostructures

Niklas Witt,[1,2,3] Siheon Ryee,[2,3] Lennart Klebl,[1,2] Jennifer Cano,[4,5]
Giorgio Sangiovanni,[1] Tim O. Wehling[2,3]

1) Institute for Theoretical Physics and Astrophysics and Würzburg-Dresden Cluster of Excellence ctd.qmat, University of Würzburg, Germany
2) I. Institute of Theoretical Physics, University of Hamburg, Germany
3) The Hamburg Centre for Ultrafast Imaging, Germany
4) Department of Physics and Astronomy, Stony Brook University, USA
5) Center for Computational Quantum Physics, Flatiron Institute, USA

Graphene-based multilayer systems serve as versatile platforms for exploring the interplay between electron correlation and topology, thanks to distinctive low-energy bands marked by significant quantum metric and Berry curvature from graphene's Dirac bands.
In this talk, we investigate Mott physics and local spin moments in Dirac bands hybridized with a flat band of localized orbitals in functionalized graphene [1]. Via hybridization control, a topological transition is realized between two symmetry-distinct site-selective Mott states featuring local moments in different Wyckoff positions, with a geometrically enforced metallic state emerging in between. We find that this geometrically controlled real-space switching of local moments and associated metal-insulator physics may be realized through proximity coupling of epitaxial graphene on SiC(0001) with group IV intercalants [1,2,3], where the Mott state faces geometrical obstruction in the large hybridization limit. Our results show that chemically functionalized graphene provides a correlated electron platform, very similar to the topological heavy fermions in graphene moiré systems [4,5] but at significantly enhanced characteristic energy scales.

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Doping monolayer graphene to the Van Hove singularity

Guangyao Miao,[1] Daniel Jansen,[1] Bilal Hawashin,[2] Julian Kleeschulte,[2] Katharina Offermann,[1] Christian Krämer,[1] Affan Safeer,[1] Abdallah Karaka,[1] Jeison Fischer,[1] Thomas Michely,[1] Michael Scherer,[2] Wouter Jolie[1]

1) II. Physikalisches Institut, Universität zu Köln, Köln, Germany
2) Theoretische Physik III, Ruhr-Universität Bochum, Bochum, Germany

Tuning correlated states in graphene is an intriguing topic, particularly since the experimental realization of superconductivity and correlated insulator states in twisted-angle bilayer graphene near the magic angle [1-3]. Such correlated phenomena have also been predicted in monolayer graphene doped to one of its van Hove singularities [4]. Motivated by this, we study the effect of Cs doping on a graphene monolayer on Ir(111). A $\sqrt{3} \times \sqrt{3}$ superstructure is observed due to the Cs intercalations between graphene and Ir(111). Further deposition of Cs on graphene leads to the formation of several surface structures with varying Cs concentrations, including adatoms, chains, stripes, and compact islands. Their morphology and electronic structures are revealed by low-temperature scanning tunneling microscopy and spectroscopy. By optimizing the dosage, we successfully tune the VHS to the vicinity of the Fermi level and observe a $2\sqrt{3} \times 2\sqrt{3}$ superstructure with respect to the graphene lattice. Possible origins of the superstructure related to many-body interactions will be discussed.

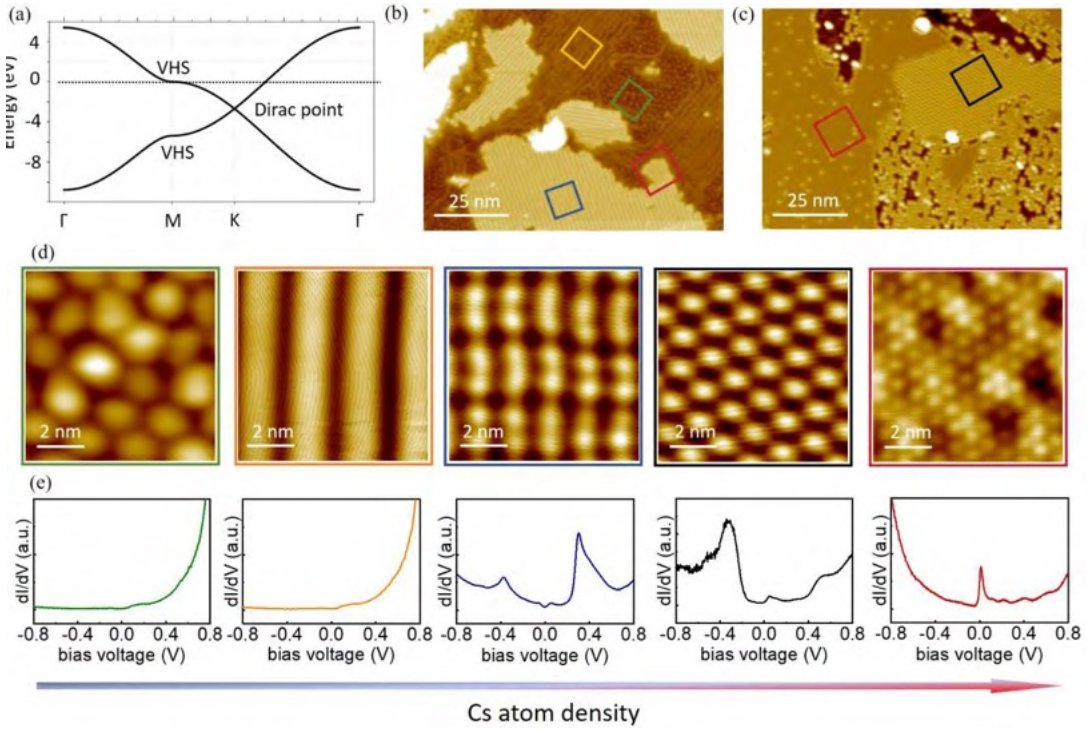

Figure 1: (a) The band structure of a graphene monolayer in the vicinity of the Van Hove singularity. (b) and (c) The large-scale STM images of increased dosages of Cs on graphene/Ir(111). (d) The zoom-in STM images of different phases of Cs on graphene/Cs/Ir(111). (e) The dI/dV spectra of the different phases shown in (d).

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Small polarons in single layer $MnBr_2$: substrate dependence and interaction with a super-moiré

Affan Safeer[1], Oktay Güleryüz[1], Guangyao Miao[1], Wouter Jolie[1], Thomas Michely[1], and Jeison Fischer[1]

[1] *II. Physikalisches Institut, Universität zu Köln, Zülpicher Straße 77, 50937 Köln, Germany*

Single-layer transition metal dihalides grown on conducting substrates were shown to host small polarons [1,2]. Here, we investigate polarons in insulating single-layer $MnBr_2$ grown by molecular beam epitaxy on three different substrates, namely graphene on Ir(110), graphene on Ir(111), and Au(111). The number densities and species of polarons observed vary strongly as a function of the substrate. For $MnBr_2$ grown on Ir(110) the largest number of polaron species is observed, namely four, of which three show clear similarities with the species observed for $CoCl_2$ on graphite [1]. Polarons in single-layer $MnBr_2$ are observed up to 300 K, indicating a remarkably high barrier to thermal hopping. They can be created, converted, and moved by the STM tip when a tunneling current flows at a proper bias voltage. The presence of an equilibrium distribution of polarons within tunneling distance to a conducting substrate implies a remarkably large magnitude of the polaron formation energy. Our findings indicate that modeling of polarons in such single-layer insulators in contact with a conducting substrate requires to take the substrate explicitly into account.
For graphene on Ir(110) as a substrate, mobile polarons in $MnBr_2$ are guided through the periodic potential imposed from the super-moiré resulting through the interaction of $MnBr_2$ with graphene and Ir(110) [3]. While this discovery is of fundamental interest, it implies that, in principle, it is possible to construct devices in which a laterally patterned potential may guide the motion of polarons.

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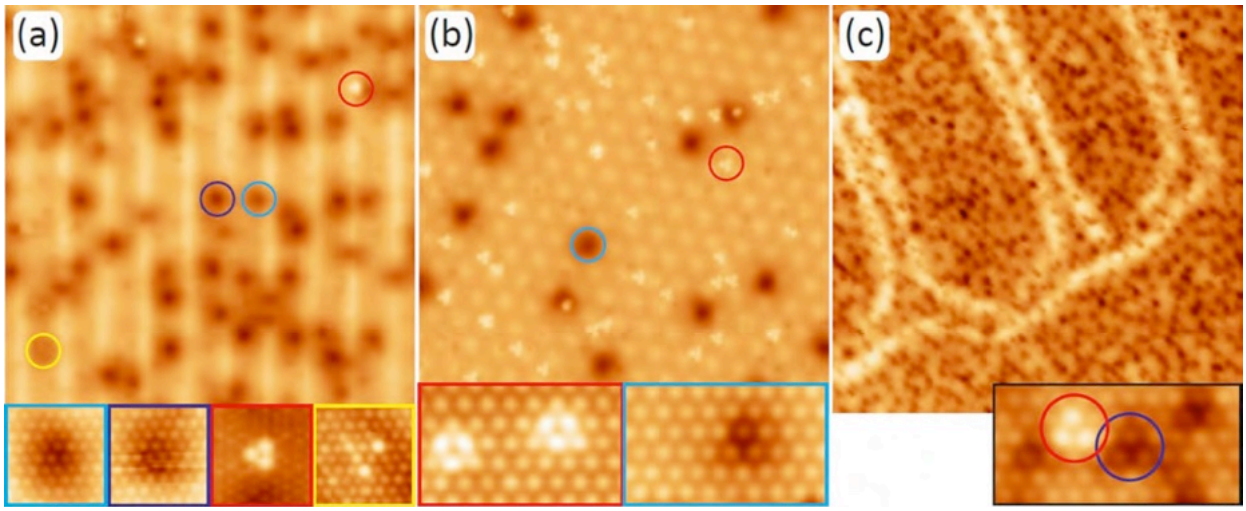

Figure: STM topographs of single layer $MnBr_2$ on (a) graphene on Ir(110), (b) graphene on Ir(111) and (c) on Au(111). The different polaron species are color-coded. The atomically resolved species present on each substrate are shown underneath the overviews. All images taken at 4.2 K. Image size in (a)-(c) is 40 nm × 40 nm.

Manipulation of Polarons in Monolayer $NiBr_2$

Anshika Mishra*, Ales Cahlik, Antti Karjasilta, Mohammad Amini, Peter Liljeroth

Department of Applied Physics, Aalto University School of Science, P.O. Box 15100, 00076 Aalto, Finland

Polarons are quasiparticles formed by the interaction of charge carriers with lattice vibrations, leading to local lattice distortions and trapped carriers. Recent studies have reported polaron signatures in the transition metal dihalide $CoCl_2$ [1,2], and demonstrated that the polarons can be created, manipulated, and erased which facilitates to study polarons in van der Waals (vdW) materials. In our work, we identify similar polaronic features in monolayer $NiBr_2$ grown on Highly Oriented Pyrolytic Graphite (HOPG) (substrate via Molecular Beam Epitaxy (MBE).

Using Scanning Tunneling Microscopy (STM) and Scanning Tunneling Spectroscopy (STS), we visualize the polarons and characterize their associated electronic states. Analogous to $CoCl_2$, we demonstrate the ability to create, erase, and move the polarons across the $NiBr_2$ islands. Spectroscopy measurements reveal localized polaronic state and a shift in the conduction band of $NiBr_2$, indicative of polaron formation during the growth process. $NiBr_2$, being a multiferroic material with similarities to NiI_2 [3], provides an intriguing system to explore the coupling between polaronic effects and multiferroic ordering in two-dimensional materials.

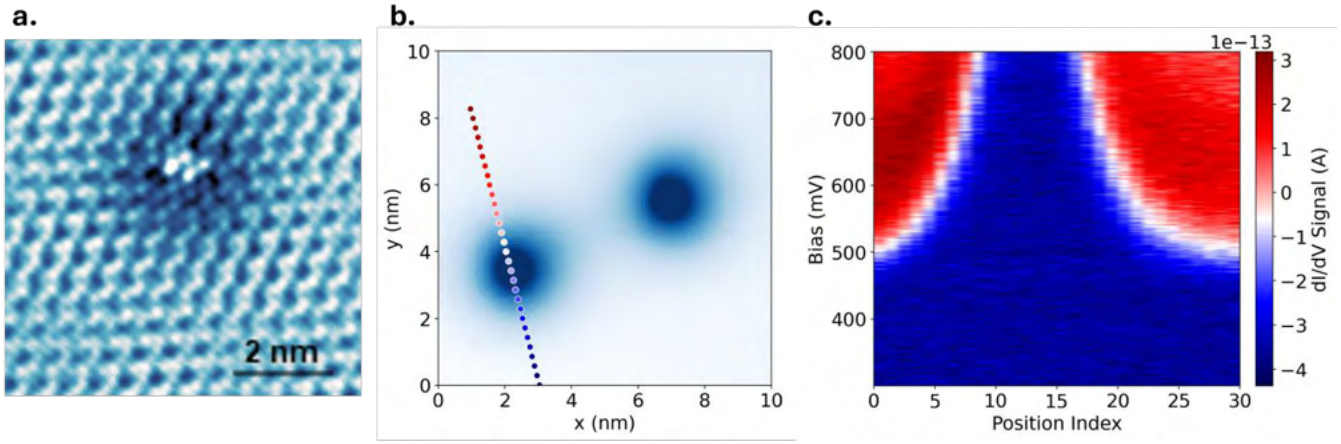

Figure 1: (a) High-resolution STM image at V_{bias} = -0.7 V (I = 7pA), resolving the localized electronic feature of the polaron. **(b)** Constant current STM image of polaron used for line spectroscopy, acquired at V_{bias} = 0.7 V (I = 3pA), with overlaid measurement points. **(c)** dI/dV spectra recorded along the line across polaron, showing band bending.

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Magnetic excitations in van der Waals quantum materials at the atomic scale

Peter Liljeroth,[1]

1) Department of Applied Physics, Aalto University, Espoo, Finland

Conventional materials hosting exotic quantum phases typically have complex atomic structures, inhomogeneities from defects, impurities, and dopants making it difficult to rationally engineer their electronic properties. This can be overcome using van der Waals (vdW) materials and their heterostructures.

I will discuss how low-temperature scanning tunneling microscopy (STM) and spectroscopy (STS) can be used to probe magnetic excitations in vdW quantum materials down to the monolayer limit and at the atomic scale. I will illustrate these capabilities through our recent results on understanding multiferroicity in van der Waals materials in the monolayer limit. Our findings provide atomic-scale evidence on the mechanism of multiferroicity in NiI_2 and related compounds and we are also able to visualize the collective excitations of the multiferroic order, electromagnons [1,2]. In addition, I will present recent work on correlated insulator 1T-$TaSe_2$, where we can resolve unconventional low-energy excitations consistent with frustrated or spin-liquid-like behavior [3]. Together, these examples demonstrate how complex magnetic structures and excitations can be probed at the atomic scale and how the versatility of vdW heterostructures enables designing emergent quantum states beyond those found in nature.

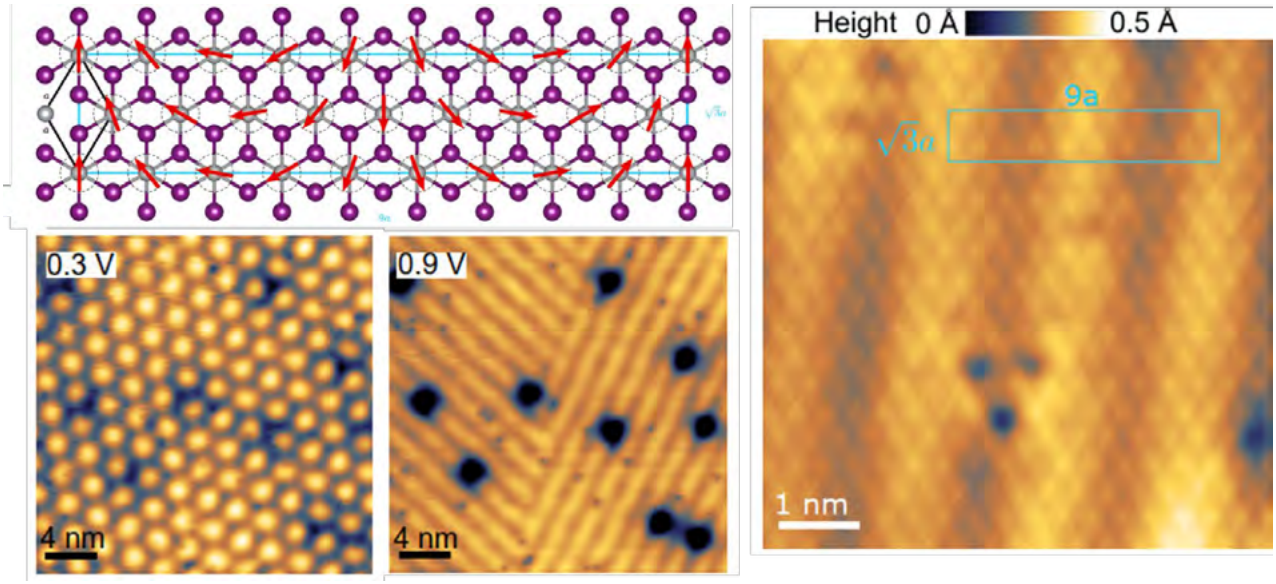

Figure 1: Imaging the magnetic spin spiral ground state in monolayer NiI_2 [1]. Depending on the bias voltage, we either resolve the moiré pattern (0.3 V) or the stripes (0.9 V) arising from the ferroelectric polarization that results from the non-collinear magnetic texture.

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Perpendicular magnetic anisotropy in a single Dy adatom ferrimagnet

Dominik Legut[1,2], Frantisek Maca[3], Itzak Halevy[4], Alexander Shick[3]

1) Charles University, Prague, Czech Republic
2) VSB Technical University of Ostrava, Ostrava, Czech Republic
3) Academy of Sciences of the Czech Republic, Prague, Czech Republic
4) Ben Gurion University of Negev, Beer-Sheva, Israel

Insert here your abstract The electronic structure and magnetism of individual Dy atoms adsorbed on ferromagnetic (Gr)/Ni(111) substrate are investigated using a combination of the density functional theory with the Hubbard-I approximation to the Anderson impurity model (DFT+U(HIA)). The divalent Dy^{2+} adatom in f^{10} configuration with [J = 8, L = 6, S = 2] is found. The values of spin M_S =3.4 μ_B, orbital M_L=5.2 μ_B, and total M_J =8.6 μ_B calculated for the Dy *f*-shell are noticeably different from the atomic second Hund's rule. There is almost zero moment on (Gr)-atoms. The ferromagnetic Ni substrate moments are anti-aligned to the Dy 4*f*-shell moment. The X-ray absorption (XAS) and magnetic circular dichroism (XMCD) spectra are calculated and can be compared to the experimental data. The magnetic anisotropy energy (MAE) is calculated from the ground state energy difference for different directions of the magnetization, E[100] - E[001] = 2.8 meV and E[010] - E[001] = 2.2 meV. This large and positive MAE can be important for ultra-high density magnetic recording. The magnetization of Dy@(Gr)/Ni(111) is tilted with respect to the (Gr)/Ni(111) substratenormal by 38° due to a competition between negative first and third order magnetic anisotropies and strong and positive second order magnetic anisotropies. Our studies assist in resolving ambiguities of conventional DFT+U applied to Dy on graphene[1]. They can provide a viable route for further investigation and prediction of the rare-earth based magnetic nanostructures.

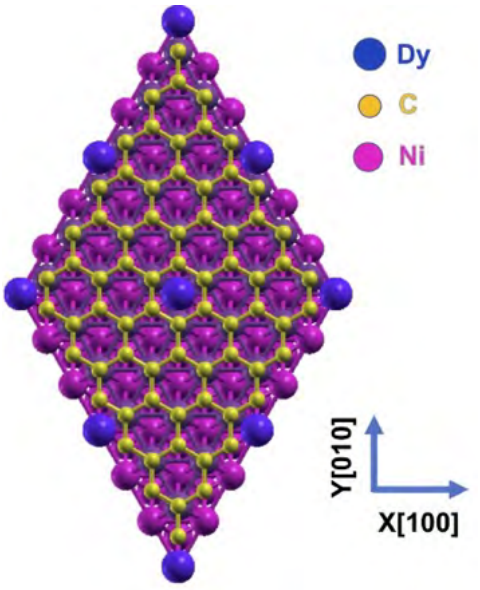

Figure 1: Supercell model for rare-earth impurity on graphene/Ni(111) (Dy@GR/Ni). Dy atoms are shown in blue, C atoms are in gold, and Ni atoms in magenta.

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Atomic manipulation on epitaxial 2D materials

Daniel Jansen,[1] Guangyao Miao,[1] Tfyeche Y. Tounsi,[1] Jan Keienburg,[1] Affan Safeer,[1] Jeison Fischer,[1] Nicolae Atodiresei,[2] Thomas Michely,[1] Hannu-Pekka Komsa,[3] Wouter Jolie[1]

1) II. Physikalisches Institut, University of Cologne, Germany
2) Peter Grünberg Institute and Institute for Advanced Simulation, Forschungszentrum Jülich, Germany
3) Faculty of Information Technology and Electrical Engineering, University of Oulu, Finland

Atomic manipulation with the tip of a scanning tunneling microscope (STM) is a bottom-up method to create novel states of matter. Combining this technique with correlated 2D materials enables us to explore tunable many-body states. Here we present two systems for atomic manipulation experiments: Fe atoms on 1H-TaS_2 on graphene (Gr)/Ir(111) and S vacancies in MoS_2 and WS_2 on Gr/Ir(111).

Fe atoms can be manipulated laterally on monolayer TaS_2 on Gr/Ir(111), enabling the assembly of artificial lattices containing tens of atoms, see Fig. 1 (a)-(b). We find two stable adsorption sites, together with local height modulations due to moiré effects. The magnetic properties of these atoms are measured using scanning tunneling spectroscopy. The most pronounced spectral feature is a zero bias (Kondo) resonance in the differential conductance, which splits in energy as a function of magnetic field.

S vacancies in monolayer MoS_2 and WS_2 on Gr/Ir(111) exhibit localized states deep in the band gap of the semiconducting host. When negatively charged, these solid-state defects host an uncompensated spin, which can be used to sense neighboring spins in its proximity [1]. Having the capability to manipulate the position of these vacancies would allow us to control their mutual interactions. For MoS_2, we found strong hybridization for closely spaced dimers, an important prerequisite for artificial lattices [2]. For WS_2, we went one step further and discovered that vacancy clusters can be manipulated laterally using the tunneling current, giving us the possibility to study their static and dynamic behavior for various spacings and symmetries, see Fig. 1 (c).

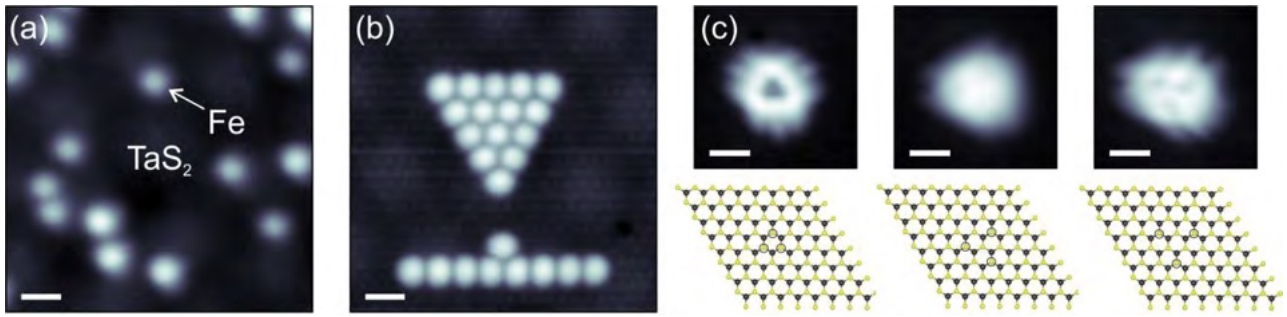

Figure 1: Atomic manipulation on 2D materials. (a) Fe atoms on TaS_2 before and (b) after manipulation. (c) STM images and corresponding ball models for vacancy trimer in various configurations. Missing S atoms are encircled. Scale bar: 1 nm.

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Atomic-Scale Mapping of Superconductivity in the Incoherent CDW Mosaic Phase of a Transition Metal Dichalcogenide

Sandra Sajan[1,], Haojie Guo[1,], Tarushi Agarwal[2], Irián Sánchez-Ramírez[1], Chandan Patra[2], Maia G. Vergniory[1,3], Fernando de Juan[1,4], Ravi Prakash Singh[2] and Miguel M. Ugeda[1,4,5]

1) Donostia International Physics Center, Paseo Manuel de Lardizábal 4, 20018 San Sebastián, Spain.

2) Department of Physics, Indian Institute of Science Education and Research Bhopal, Bhopal 462066, India.

3) Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany.

4) Ikerbasque, Basque Foundation for Science, 48013 Bilbao, Spain.

5) Centro de Física de Materiales, Paseo Manuel de Lardizábal 5, 20018 San Sebastián, Spain.

The emergence of superconductivity in the octahedrally coordinated (1T) phase of TaS_2 is preceded by the intriguing loss of long-range order in the charge density wave (CDW). Such decoherence, attainable by different methods, results in the formation of nm-sized coherent CDW domains bound by a two-dimensional network of domain walls (DW) - mosaic phase -, which has been proposed as the spatial origin of the superconductivity. Here, we report the atomic-scale characterization of the superconducting state of 1T-TaSSe, a model 1T compound exhibiting the CDW mosaic phase. We use high-resolution scanning tunneling spectroscopy and Andreev spectroscopy to probe the microscopic nature of the superconducting state in unambiguous connection with the electronic structure of the mosaic phase. Spatially resolved conductance maps at the Fermi level at the onset of superconductivity reveal that the density of states is mostly localized on the CDW domains compared to the domain walls, which suggests their dominant role in the formation of superconductivity. This scenario is confirmed within the superconducting dome at 340mK, where superconductivity is fully developed, and the subtle spatial inhomogeneity of the superconducting gap remains unlinked to the domain wall network. Our results provide key new insights into the fundamental interplay between superconductivity and CDW in these relevant strongly correlated systems.

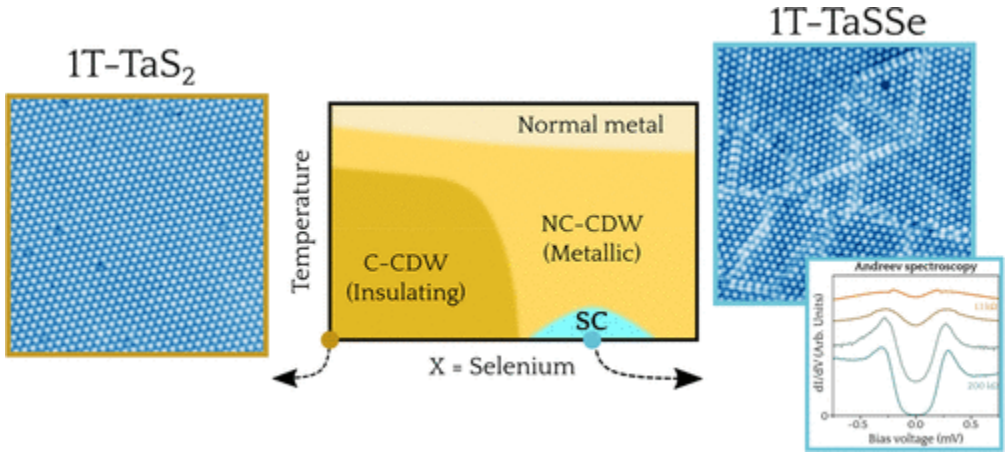

Figure 1: Superconductivity in Mosaic CDW in 1T-TaSSe

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DAY 3

7:00 - 9:00	**Breakfast**

Chair: **Matthias Batzill**

9:00 - 9:30	Invited: **Jeison Fischer** - Epitaxial growth pathways to magentic order in novel 2D materials
9:30 - 9:50	Contributed: **David Serrate** - Atomic scale demonstration of ferromagnetism in a single layer FeCl2 on Au(111)
9:50 - 10:20	Invited: **Marin Petrović** - Beyond pristine monolayer borophene: towards functionalization and bilayers
10:20 - 10:40	Contributed: **Patrick Seleš** - Fast synthesis of large hBN domains on commerical nickel foils by UHV-CVD
10:40 - 11:00	Contributed: **Marjolaine Cornu** - Heteroepitaxial growth of 2D BN films on Ni(111) by CVD with controlled thicknesses
11:00 - 11:30	**Coffee**

Chair: **Matthias Batzill**

11:30 - 12:00	Invited: **Irene Groot** - Growth of two-dimensional materials on liquid metal catalysts
12:00 - 12:20	Highlight: **Lars Mohrhusen** - TiS2-based 2D nanocatalysts under reactive conditions
12:20 - 12:40	Contributed: **Thais Chagas** - Electronic structure and edge states in the 2D kagome Ta2S3 on Au(111)
12:40 - 12:55	**Conference Photo**
12:55 - 14:10	**Lunch**
14:10 - 19:00	**Excursion**




19:00 - 20:30	**Dinner**
20:30 - 22:00	Poster Session

Epitaxial Growth Pathways to Magnetic Order in Novel 2D Materials

Jeison Fischer

Institute of Physics II, University of Cologne, Germany

The discovery of intrinsic magnetism in exfoliated 2D materials marked a pivotal advance, demonstrating that long-range magnetic order can persist in the atomically thin limit. While mechanical exfoliation—born in the graphene era—has unlocked access to several 2D magnetic phases, it is inherently limited to bulk-stable structures, restricting exploration of metastable or non-bulk-related materials. Molecular beam epitaxy (MBE) overcomes this limitation by enabling precise, layer-by-layer growth of single-layer materials that are structurally and electronically distinct from their bulk counterparts [1]. In my talk, I will highlight how tailored epitaxial growth pathways on graphene/Ir surfaces serve as a powerful platform for engineering novel 2D materials with emergent magnetic properties.

First, epitaxial growth of chromium sulfide at the 2D limit yields single-layer Cr_2S_3-2D (Fig. 1a), featuring a five-atom-thick S–Cr–S–Cr–S stack with octahedrally coordinated Cr atoms. This ultimate thin NiAs-type structure is fully covalent and lacks van der Waals gaps [2]. Using spin-polarized scanning tunneling microscopy (STM) and X-ray magnetic circular dichroism, we determine the magnetic ground state of Cr_2S_3-2D, revealing in-plane ferromagnetic coupling with out-of-plane moments and antiferromagnetic coupling between Cr planes, thereby realizing the first single-layer 2D material with type-A antiferromagnetic order (Fig. 1b).

Second, epitaxial growth of iron sulfide results in metastable tetragonal Fe_2S_2, structurally identical to bulk mackinawite. Vacuum annealing induces a phase transformation to a single-layer hexagonal Fe_2S_2 phase that is structurally distinct from conventional transition metal chalcogenides polymorphs. In this 2D exclusive hexagonal structure, h-Fe_2S_2-2D, Fe atoms occupy tetragonally coordinated sites, characteristic of CuI-type structure. Spin-polarized STM on h-Fe_2S_2-2D islands (Fig. 1c) reveals that the moments are not collinear within the plane. We map the in-plane components of two distinct magnetic configurations and find that the moments are confined to the 2D plane, forming an antiferromagnetic 120° Néel state (Fig. 1d) and a 2Q in-plane spin-spiral.

These results highlight the potential of epitaxial growth to access novel structural and magnetic phases, offering a complementary route to exfoliation for exploring 2D materials with unique properties.

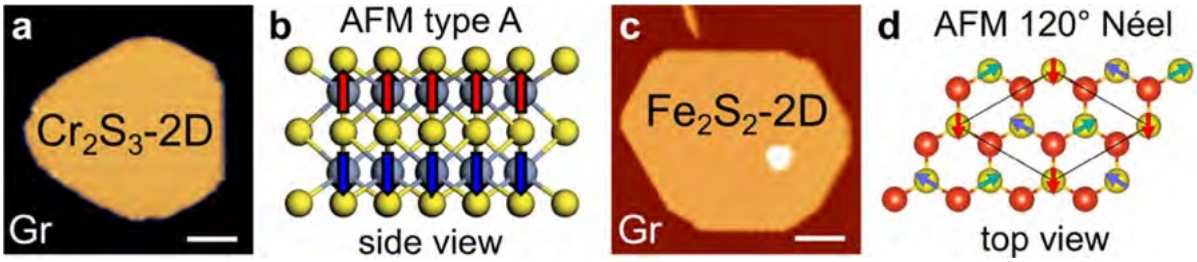

Figure 1: Isolated nanometer size islands of Cr_2S_3-2D (a) and h-Fe_2S_2-2D (c). Schematics of the spin structures overlaid ball models (b,d). Scale bar: 10 nm (a) and 5 nm (c).

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Atomic scale demonstration of ferromagnetism in a single layer $FeCl_2$ on Au(111)

David Serrate,[1,2] Adriana Candia,[3,4] Eliecer Peláez-Sifonte,[1] Amitayush Jha Thakur,[3] Sebastien E. Hadjadj,[3] Samuel Kerschbaumer,[3] Aymeric Saunot,[3] Martina Corso,[3] Maxim Ilyn,[3] Jorge Lobo Checa,[1,2] Celia Rogero.[3]

1) Instituto de Nanociencia y Materiales de Aragón, CSIC-Universidad de Zaragoza, E-50009, Spain
2) Departamento de Física de la Materia Condensada, Universidad de Zaragoza, E-50009, Spain
3) Centro de Física de Materiales, CSIC-UPV/EHU, E-200018, Spain
4) Laboratorio de Microscopias Avanzadas, Universidad de Zaragoza, E-500018, Spain.

The ability of two-dimensional (2D) materials to maintain long-range magnetic ordering has significant technological implications. They can induce magnetic functionalities, such as spin filtering or spin current generation, when incorporated into van der Waals (vdW) heterostructure stacks. $FeCl_2$ is a promising single-layer material with robust ferromagnetism that can be easily grown by molecular beam epitaxy on Au(111). However, its magnetic properties and the influence of the underlying Au(111) substrate are not fully understood [1,2]. To include this material into the palette of vdW crystals, it is important to unambiguously confirm their magnetic ground state experimentally. Using spin-polarized STM, tunnelling spectroscopy, and angle-resolved photoemission spectroscopy, we investigated this material and found that mobile atomic scale defects play a primary role in the electronic gap and spin density distribution. We report on the dependence of the spin density of a single $FeCl_2$ slab on Au(111) as a function of magnetic field and the position of atomic-scale defects using SP-STM. We find that the local magnetization of each $FeCl_2$ flake corresponds to that of a soft ferromagnet with pronounced out-of-plane magnetocrystalline anisotropy, with nearly squared magnetization loops and coercive fields of a few tens of mT (few hundred Oe). We will also discuss recent findings on the magnetic coupling between contiguous $FeCl_2$ slabs.

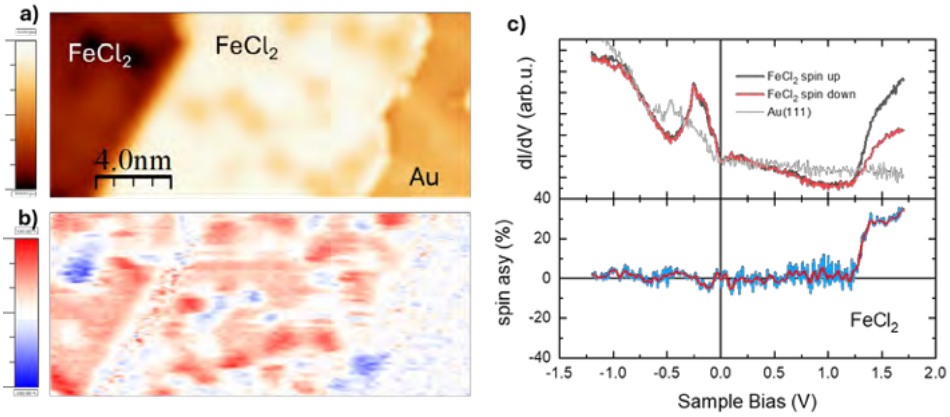

Figure 1: a) STM topography image of a $FeCl_2$ single layer on Au(111) (1V, 15 pA). b) Spin contrast map in differential conductance (dI/dV) of the same region retrieved with an out-of-plane sensitive bulk Cr-tip (1.5V, 100 pA, modulation 10 mV rms). c) Averaged dI/dV spectra of $FeCl_2$ with magnetization parallel (red) and antiparallel (black) to the tip's magnetic moment. The bottom panel shows the computed spin asymmetry as a function of energy (blue error bars represent the statistical standard deviation).

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Beyond pristine monolayer borophene: Towards functionalization and bilayers

Marin Petrović

Centre for Advanced Laser Techniques, Institute of Physics, Zagreb, Croatia

Borophene, a polymorphic two-dimensional (2D) form of boron, is an exciting atomically-thin material with many advanced properties [1], some of which surpass the properties of its carbon-built cousin, graphene. Even though significant advancements have been made in the research of borophene, it remains challenging to improve its stability, perform targeted functionalization and fabricate more complex systems such as bilayers and heterostructures. In this talk, our recent microscopic, spectroscopic and computational results of borophene on Ir(111) will be presented tackling some of these open issues. Synthesis of borophene has been conducted either by a dissolution-segregation route from gaseous borazine precursor [2] or by molecular beam epitaxy from a solid boron rod. The first approach results in an extended single-layer borophene [3,4], suitable for post-growth functionalization, while the second one allows surpassing of the monolayer limit and fabrication of borophene with bilayer characteristics. For the monolayer samples, intrinsic properties of pristine borophene were modified by adsorption of lithium atoms which readily induce changes of borophene's electronic structure and morphology. The dominant factors which govern these modifications are charge donation of lithium and high chemical reactivity of borophene. For the fabricated bilayer samples, distinct features were detected in the valence band structure and core levels which can be correlated with the formation of a well-defined, electronically decoupled boron sheet. Overall, the presented results provide insights into strategies for the fabrication of more complex boron-based 2D systems and pinpoint to promising directions and challenges in fundamental and applicative studies of borophene.

This work was conducted in collaboration with M. Horn von Hoegen, A. Locatelli, P. Moras, T. Michely, Y. Gohda and their group members, as well as other members of the SIMAT group at the IoP Zagreb.

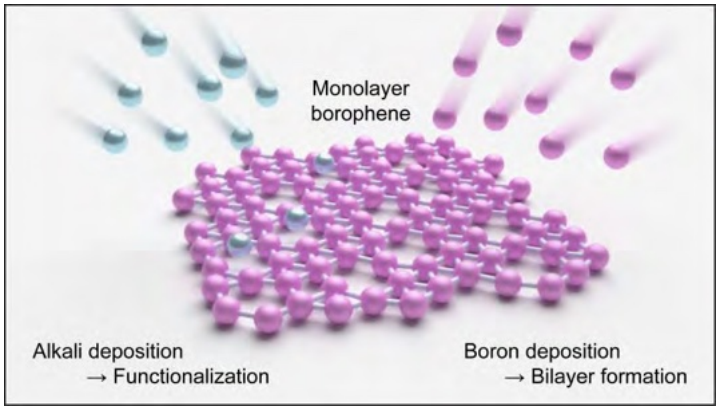

Figure 1: Schematic illustration of monolayer borophene, which can be functionalized by the deposition of alkali atoms (left hand side) or can be transformed into a bilayer by deposition of additional boron atoms (right hand side).

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Fast synthesis of large hBN domains on commercial nickel foils by UHV-CVD

Patrick Seleš,[1] Martina Lihter,[1] Sabina Špoljar[1], Borna Radatović[1], Martin Vesely,[2] Marin Petrović[1]

1) Centre for Advanced Laser Techniques, Institute of physics, Zagreb, Croatia
2) University of Chemistry and Technology, Prague, Czech Republic

Hexagonal boron nitride (hBN) is a technologically interesting 2D material with exceptional chemical and physical properties [1]. Chemical vapor deposition (CVD) on metal substrates is often chosen for the growth of hBN since it is a scalable synthesis route, which provides samples of high structural quality [2]. Even though polycrystalline metal foils represent suitable and affordable substrates for the CVD process, controlled growth on them remains challenging because of complex substrate-precursor interactions [3].

Here, we report a rapid approach for synthesizing hBN on commercial nickel foils by ultra-high vacuum CVD (UHV-CVD) using borazine as a precursor, combined with ex-situ microscopy (SEM, AFM) and spectroscopy (EDS, ToF-SIMS) techniques for sample characterization. A short electron-beam annealing step is first used to recrystallize the Ni foils, which produces large, well-defined crystal grains. By systematically varying growth temperature and precursor pressure, we observe distinct hBN morphologies, reflecting their strong dependence on substrate crystallography and growth kinetics. With optimized growth conditions we were able to produce large hBN islands with lateral dimensions reaching hundreds of micrometers. In addition to hBN formation, boron-rich crystallites are observed, whose density and size clearly depend on temperature, cooling rate, and grain orientation. Analysis reveals that boron most likely dissolves into the Ni substrate at elevated temperatures and segregates toward the surface upon cooling, competing with hBN formation. These findings provide insight into the kinetic and thermodynamic factors governing hBN growth on Ni foils and offer guidance for scalable synthesis.

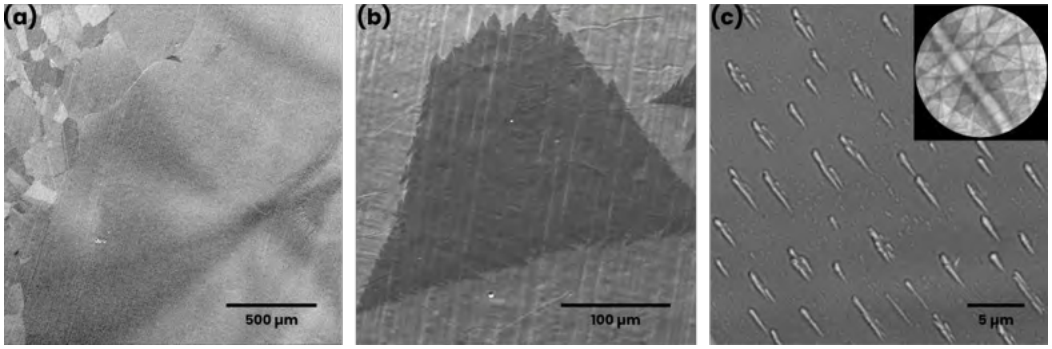

Figure 1: Overview of hBN growth on annealed Ni foils by UHV-CVD: (a) recrystallized Ni grains after electron-beam annealing, (b) large hBN island grown on a single Ni grain, and (c) boron-rich crystallites formed after synthesis at high temperatures.

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Heteroepitaxial growth of 2D BN films on Ni(111) by CVD with controlled thicknesses

M. Cornu[1], L. Tailpied[1], A. Andrieux-Ledier[2], C. Grekobi[1], J.Lagrave[1], F. Fossard[1], J.S. Mérot[1], L. Sponza[1], J.M. Decams[3], A. Loiseau[1]

[1] *Université Paris-Saclay, ONERA, CNRS, Laboratoire d'Etude des Microstructures, F-92322 Châtillon, France*
[2] *Université Paris-Saclay, ONERA, DPHY, F-92322 Châtillon, France*
[3] *Annealsys, 139 rue des Walkyries, 34000 Montpellier, France*

Among 2D materials, boron nitride (BN) has attracted a great interest over the past years due to its remarkable properties. It is an insulator with a large band gap (around 6 eV), a high chemical and thermal resistance and an atomically plane surface with a lattice parameter very close to the one of graphene. This makes it a key material for the fabrication of Van der Waals heterostructures and devices in optics, electronics and spintronics [1][2]. Up to now, the majority of the devices or proof of concept have been realized with hBN flakes mechanically exfoliated from crystals. This method provides flakes of high quality but with a limited surface area. In order to integrate boron nitride in nano-devices, there is a need for large-scale synthesis. On-going researches are done with techniques such as MBE, ALD or CVD but so far a real control of the thickness and film quality has not been reached [3].

In this context we develop a synthesis route of sp^2-hybridized BN films by CVD [4]. The growth is done in a rapid thermal processing system with halogen lamps under primary vacuum. We use borazine as a precursor on a Ni(111) pseudo-substrate for an epitaxial growth of BN multilayers. The films are then characterized from the mm to the nm scale by TEM in-plane and in cross-section, SEM, AFM, XPS and statistical Raman microscopy, either on the growth substrate or after being transferred on a SiO2/Si substrate. We succeeded in synthesizing and transferring films of several mm^2 that are homogeneous and crystallized. By varying growth parameters such as the nickel substrate thickness, the borazine partial pressure or the time of exposure, we obtained samples with thicknesses varying from 2 to 20 layers. The different characterizations provide insights into the influence of each parameter and helps to understand the growth mechanism of BN films on Ni(111) by CVD, which is essential for achieving controlled synthesis of BN films.

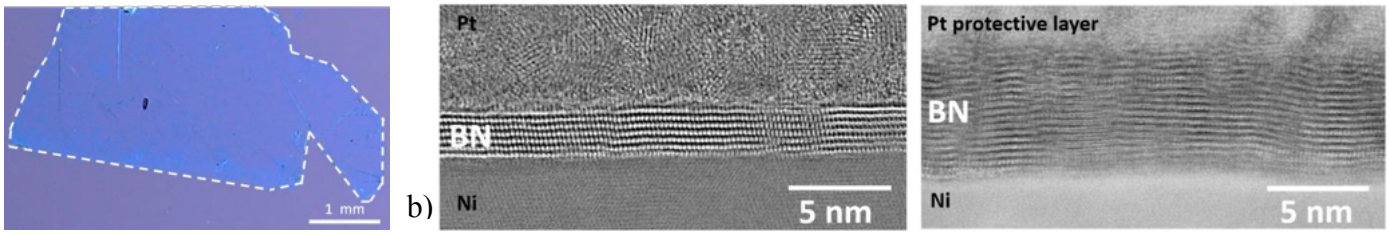

Figure 1: a) Optical microscopy image of a BN film, 8-10 layers thick, transferred on 90 nm SiO_2/Si substrate. b) STEM images of cross-section of BN films with various thicknesses (200kV, iDPC mode)

References

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Growth of Two-Dimensional Materials on Liquid Metal Catalysts

Irene M.N. Groot[1]

1) Leiden Institute of Chemistry, Leiden University, Einsteinweg 55, 2333 CC Leiden, the Netherlands

Two-dimensional materials have unique electronic, magnetic, optical, and mechanical properties that differ significantly from their bulk counterparts. They show promise for various applications, such as (opto)electronics, photonics, or novel catalysts [1-4]. The growth of 2D materials via chemical vapor deposition is the most promising for use at an industrial scale due to its low cost and scalability. However, the growth of large-scale, defect-free 2D materials still forms a bottleneck for their application. Liquid metal catalysts can be the solution to this problem. In 2012, Geng et al. demonstrated for the first time that graphene can be grown on a liquid copper substrate [5].

To be able to shed light on the growth kinetics of graphene on liquid copper, we developed a dedicated CVD reactor to investigate this process in real time, employing synchrotron X-ray-based techniques, optical microscopy, and Raman spectroscopy, during the actual growth process [6]. We showed that monitoring the growth process in situ enabled us to tailor the growth to obtain large-scale, single-crystalline, defect-free single layers of graphene with superior properties [7,8].

In this talk, I will discuss the growth of graphene on various liquid metal substrates, but will also show that we can use our dedicated reactor and novel operando analysis techniques to investigate other 2D materials such as h-BN and GaN.

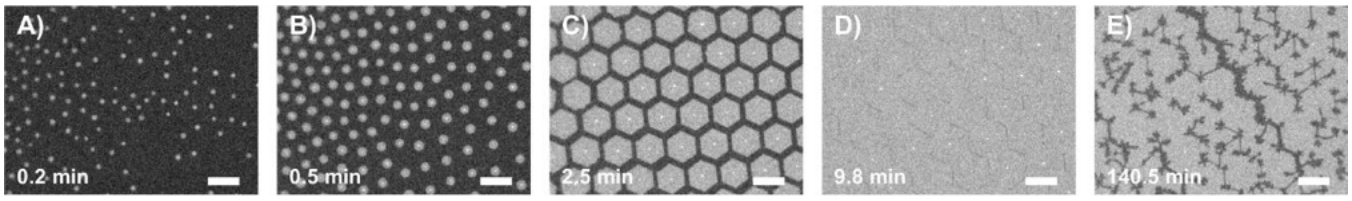

Figure 1: Optical microscopy images of graphene growth on liquid copper.

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TiS_2-based 2D nanocatalysts under reactive conditions

Niko Kruse[1], Marc Kobbenbring[1], Justin Klimek[1], Aaron von Seggern[1], Martin Hedevang[2], Sergi Campos Jara,[2] Jeppe V. Lauritsen[2], and Lars Mohrhusen[1]

1) Carl von Ossietzky University of Oldenburg, D-26129 Oldenburg, Germany

2) Aarhus Universitet, 8000 Aarhus, Denmark

To overcome challenges in the energy transition, heterogeneous (photo)catalysis is a key technology. Our target is to develop sustainable noble-metal free (photo-)catalysts by combining reduceable oxides with 2D materials, based on the surface-science approach: To overcome experimental limitations under technical conditions, we investigate model systems by using well-defined (single crystal) samples from ultra-high vacuum to operando conditions (usually few mbars). Combining insights from spectroscopy, microscopy and reactivity studies can gain a comprehensive picture down to the atomic level.[1,2,3]

To replace critical elements such as platinum group metals (PGM) and many other transition metals, Titanium is an excellent candidate due to its availability and attractive sustainability footprint. Motivated by the reactivity of electron-rich Ti sites such as defects in TiO_2 for small molecule conversion and greenhouse gas activation,[4,5], herein recent results on hybrid Ti-based model systems for (photo-)catalytic reactions will be presented, especially combinations of oxides and nanostructured 2D nanosulfides. For example, 2D TiS_2 nanoparticles on metal and oxide surfaces will be introduced as potential candidates for future photocatalytic applications.[6]

The synthesis chemical potential of S was identified as the key to tailor the shape and edge structure of single layer TiS_2 particles on Au(111).[6] These particles exhibit a bright edge feature in scanning tunneling microscopy similar to the quasi-metallic edge of MoS2.[6] In comparison to Au(111), the TiS_2 particles appear to interact more strongly with oxide substrates, here rutile TiO_2 (110), leading to more elongated shapes and a limited thermal stability. NEXAFS allows a chemically sensitive identification of structural features across both substrates. Finally, the surface chemistry of titanium sulfides was studied in reductive (molecular H_2) and mildly oxidative (H_2O) atmospheres in a wide temperature range, indicating a high stability of the TiS basal planes under catalytically relevant conditions.

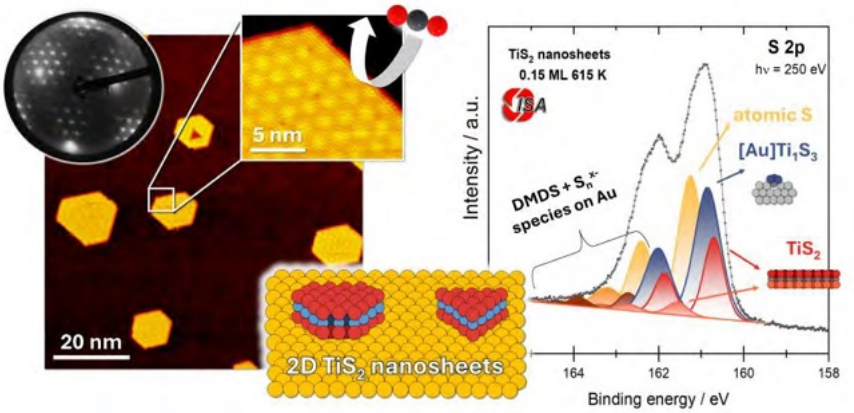

Figure 1: Graphical overview of 2D TiS_2 nanoparticles on Au(111) surfaces in low-energy electron diffraction (LEED), scanning tunnelling microscopy (STM) and X-ray photoelectron spectroscopy (XPS).

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Electronic structure and edge states in the 2D kagome Ta_2S_3 on Au(111)

Alice Bremerich,[1] Dina Wilks,[1] Christoph Schuster,[1] Pedro H. Rezende-Goncalves,[2,3] Marcin Rosmus,[2] Tomasz Sobol,[4] Edyta Beyer,[4] Barbara Wolanin,[4] Alessia Bardazzi,[1] Samuel M. Vasconcelos,[5] Alan C. R. Souza,[3] Catherine Grover,[1] Kai Mehlich,[1] François Bertrand,[6] Chiara Bigi,[6] Andrés F. Santander-Syro,[2] Mario S. C. Mazzoni,[3] Michael Rohlfing,[5] Carsten Busse,[1] Thais Chagas[1]

1) Department Physik, Universität Siegen, Siegen, Germany
2) Institut des Sciences Moléculaires d'Orsay, Université Paris-Saclay, Orsay, France
3) Departamento de Física, Universidade Federal de Minas Gerais, Belo Horizonte, Brazil
4) SOLARIS National Synchrotron Radiation Centre, Jagiellonian University, Krakow, Poland
5) Institute of Solid State Theory, Universität Münster, Münster, Germany
6) Synchrotron SOLEIL, Saint-Aubin, France

The kagome structure is an important model system in quantum physics as it combines topology and correlations. It constitutes the most frustrated 2D magnetic lattice, where the magnetic moments condense into a spin liquid at low temperature. The characteristic kagome bands consist of a Dirac cone that gives rise to massless Dirac fermions with high mobility and a flat band that, on the contrary, generates infinitely massive ones. The presence of these bands and their unique properties can give rise to exotic many-body states, including magnetism, superconductivity, and Wigner crystallization.

In this work, we investigate the two-dimensional Ta_2S_3 kagome phase on Au(111) using scanning tunneling microscopy (STM), angle-resolved photoemission spectroscopy (ARPES), and density functional theory (DFT). This novel phase was synthesized by molecular beam epitaxy (MBE) through the evaporation of Ta onto Au(111), followed by annealing in an H_2S atmosphere used as the sulfur source. STM measurements reveal bright island edges, indicative of an enhanced local density of states. Additionally, we observe a strong dependence of atomic contrast on tunneling conditions, pointing to a complex electronic band structure near the Fermi level. Finally, we analyze the impact of growth parameters on defect formation.

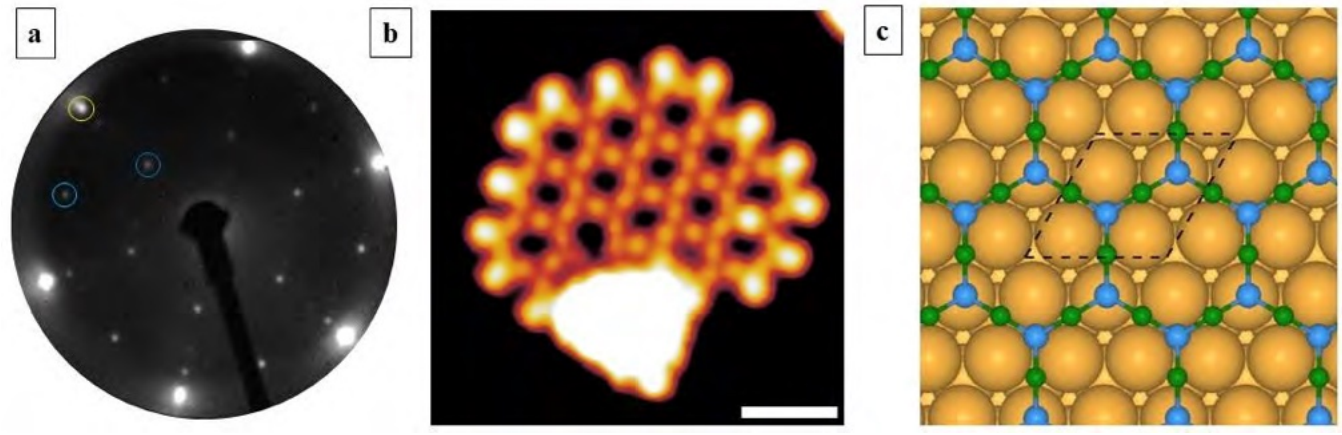
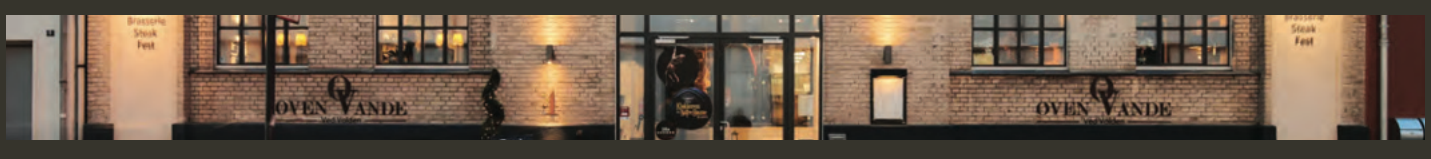


Figure 1: (a) LEED image of a large-scale kagome sample (blue circles) on Au(111) (yellow circles). Measured at 48 eV. (b) Kagome island. The contrast was enhanced to highlight the lattice of the Kagome structure. Scale bar: 1 nm, U = -0.9 V, I = 0.5 nA. (c) Structural model of the kagome lattice on Au(111) (top view). The black dashed line highlights the unit cell. Au atoms are shown in gold, Ta in blue and the S in green.

DAY 4

7:00 - 9:00	**Breakfast**
	Chair: **Oliver Gröning**
9:00 - 9:45	Keynote: **Roser Valentí** - Emergent correlations and topology in van der Waals heterostructures
9:45 - 10:05	Highlight: **Maarten Goesten** - Quasiatomic pore bands
10:05 - 10:25	Contibuted: **Benjaman Lowe** - Strong electron correlations in 2D kagome metal-organic frameworks
10:25 - 10:45	Contributed: **J. Aaron Mendoza Rodarte** - Gold-Assisted Exfoliation of 2D Materials for Vacuum-Compatible Spectroscopy
10:45 - 11:15	**Coffee**
	Chair: **Oliver Gröning**
11:15 - 11:35	Contributed: **Dina Wilks** - Electronic structure of multiferroic SnSe from monolayer to bulk
11:35 - 11:55	Contributed: **Ezequiel Tosi** - Thermally driven α-β phase transition and alloy formation in SnSe/Au(111)
11:55 - 12:15	Company: **Saumya Mukherjee (SPECS)** - Multifunctional momentum microscope for 2D material research
12:15 - 12:35	Company : **Vasileios Theofylaktopoulos (Heidelberg Instruments)** - Strain it, sculpt it, cut it: thermal scanning probe lithography in 2D materials research
12:35 - 14:05	**Lunch**
	Chair: **Yuriy Dedkov**
14:05 - 14:35	Invited: **Hélène Seiler** - Probing electronic disorder in nanomaterials with coherent two-dimensional spectroscopy
14:35 - 15:05	Contributed: **Šimun Mandić** - Charge and resonant energy transfer in hybrid organic-TMDs heterostructures
15:05- 15:35	
	Chair: **Yuriy Dedkov**
15:35 - 16:05	Invited: **Amilcar Bedoya-Pinto** - Recent developments in epitaxially grown 2D magnets: from 2D-XY systems to high-Tc magnets driven by self-intercalation
16:05 - 17:25	Contributed: **Antti Karjasita** - Evidence of multiferrocity in monolayer NiBr2
17:25 - 17:45	Contributed: **Xue Li** - Ferroelectric domain boundaries as internal quantum wells in van der Waals TMDs

19:30 - 22:00 **Conference Dinner**



Emergent Correlations and Topology in van der Waals Heterostructures

Roser Valentí[1]

1) Institut für Theoretische Physik,
Goethe Universität Frankfurt,
60438 Frankfurt am Main, Germany

The controlled stacking, twisting, and straining of two-dimensional van der Waals materials has opened new avenues for realizing correlated and topological quantum phases. In such heterostructures, interactions between layers can give rise to emergent behavior not present in the individual constituents, including correlated metals, unconventional magnetism, and topological superconductivity. In this talk, I will outline theoretical approaches for modeling these systems and highlight representative examples that demonstrate the richness of their electronic and magnetic properties [1-7], with connections to recent experimental findings.

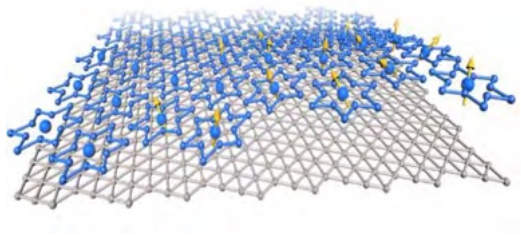


Figure 1: 1T-1H-TaS_2 Heterostructure (from [4])

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[7] Yang *et al.* Nature Materials **22**, 50 (2023)

Quasiatomic Pore Bands

Laura Berg,[1] Maarten Goesten,[1]

1) Department of Chemistry, Aarhus University, Aarhus, Denmark, 8000

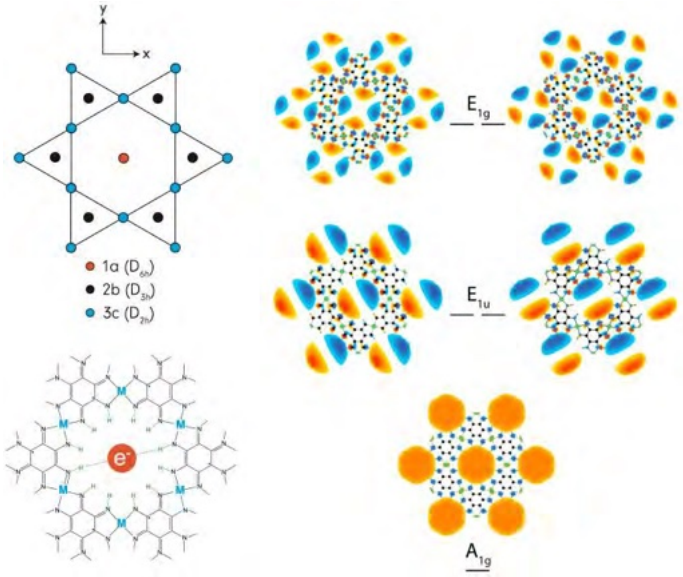

Figure 1: *Left top*. Wyckoff positions in the hexagonal lattice of $M_3(HIB)_2$, with the corresponding sitesymmetry group type in brackets. *Left bottom*. Detailed drawing showing the radicals as well as the inner pore hydrogens, in green. The hydrogens form a tubular shell around an electron at the Wyckoff 1a position, which corresponds to an occupied pore band. *Right*. Computed charge density of different pore states in $Ni_3(HIB)_2$, colored by the sign of the underlying orbitals to indicate symmetry. The labels indicate different irreducible representations of the D_{6h} crystallographic point group.

Using first-principles calculations, we predict the hexaiminobenzene (HIB) family of layered 'graphiteanalogue' metal– organic frameworks (MOFs) to host a robust and strongly bound electron quasiatom in its tubular pores. This floating state is similar to the interlayer state that was found to be crucial to superconductivity in graphite intercalation compounds,[1-2] but it is stabilized by the framework's hydrogen-lined pore walls. Moreover, as shown in the figure, the quasiatom brings its own s, p, and d orbitals, with the s-type levels computed to lie as little as $\sim$ 100 meV above the Fermi level. This means they can be controllably occupied through gating or moderate pressure. When the MOF is magnetic, we predict an energy splitting of pore-centered spin bands, with a more contracted charge density for the minority spin species. This allows for the pore to be used as a spin filter. The quasiatomic pore states are also computed to be robust in the face of common structural distortions in which layers deviate from an ideal eclipsed stacking.

Ongoing work in Aarhus currently looks at the experimental characterisation of this new quantum state, and aims to outline the first design principles for an orbital-selective use of metal-organic pore space.

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Strong electron correlations in 2D kagome metal-organic frameworks

B. Lowe,[1,2,3] B. Field,[1,2,4,5] D. Kumar[1,2], J. Hellerstedt,[1,2] J. Ceddia,[1,2] H.L. Nourse,[6,7] Y. Yin,[1,2] D.M. Cerrada,[1,2] O. Stetsovych,[3] A.P. Solé,[3] A. Domínguez-Celorrio,[1,2] S.M. Griffin,[4,5] P. Jelínek,[3] B.J. Powell,[7] N.V. Medhekar,[2,8] A. Schiffrin[1,2]

1) School of Physics & Astronomy, Monash University, Clayton, Victoria 3800, Australia
2) ARC Centre of Excellence in Future Low-Energy Electronics Technologies, Monash University, Clayton, Victoria 3800, Australia
3) Institute of Physics of the Czech Academy of Sciences, Cukrovarnická 10/112, 162 00 Prague, Czech Republic
4) Materials Science Division, Lawrence Berkeley National Laboratory, Berkeley, California 94720, USA
5) Molecular Foundry, Lawrence Berkeley National Laboratory, Berkeley, California 94720, USA
6) Quantum Information Science and Technology Unit, Okinawa Institute of Science and Technology Graduate University, Onna-son, Okinawa, Japan
7) School of Mathematics and Physics, The University of Queensland, Brisbane, QLD, Australia
8) Department of Materials Science and Engineering, Monash University, Clayton, Victoria 3800, Australia

Two-dimensional (2D) and layered electronic materials characterized by a kagome lattice have attracted attention for their potential to host strongly correlated electronic phases. Here, direct experimental evidence of strong electron–electron Coulomb interactions in a 2D metal–organic framework (MOF) is reported. The MOF consists of 9,10-dicyanoanthracene (DCA) molecules arranged in a kagome structure via coordination with copper (Cu) atoms. Via scanning probe microscopy, we demonstrate the presence of local magnetic moments at DCA and Cu sites of the MOF on metallic Ag(111) – a signature of electron correlations within the MOF,[1] and the ability to control the coupling of the MOF spins with the surface.[2] In an electronically decoupled environment provided by a monolayer of insulating hexagonal boron nitride (hBN), we directly observe a ~200 meV bandgap associated with the formation of a Mott insulating phase within the MOF.[3] Furthermore, we can control metal-insulator transitions by changing electron filling of the kagome bands. These are promising findings for controlling correlated electronic phases in 2D metal-organic materials with the potential for nanoelectronics and spintronics technologies.

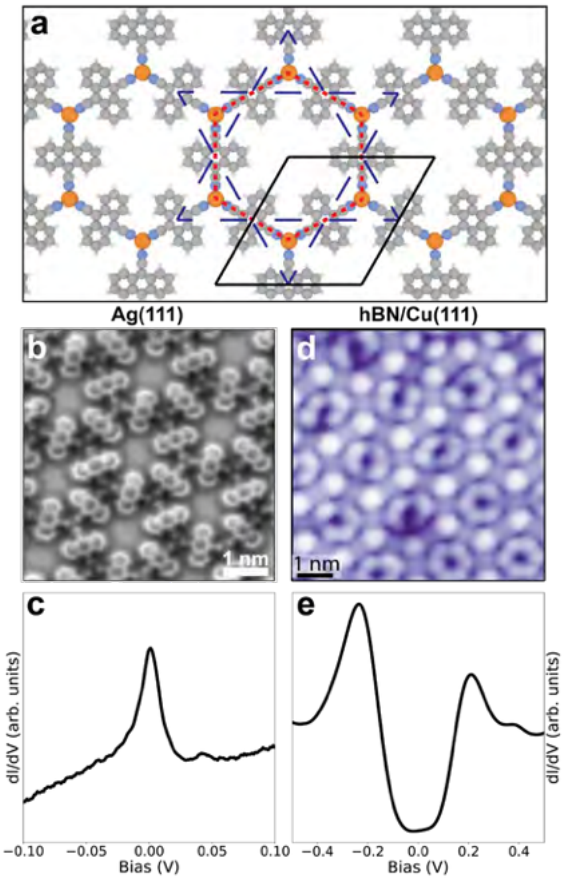

Figure 1: a Structure of DCA-Cu kagome MOF. **b,c** ncAFM image and STS spectrum acquired on Ag(111), where zero-bias peak revealed local magnetic moments. **d,e** STM image and STS spectrum acquired on hBN, revealing a gapped Mott insulating phase.

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Gold-Assisted Exfoliation of 2D Materials for Vacuum-Compatible Spectroscopy

J. Aaron Mendoza-Rodarte[1], Zhiying Dan[1], and Antonija Grubišić-Čabo[1]

1) Zernike Institute for Advanced Materials, University of Groningen, The Netherlands.

Gold-assisted exfoliation has emerged in recent years as a powerful route to obtain large-area monolayers of two-dimensional (2D) materials [1]. Large size, often on mm scale, monolayer uniformity and the presence of a metallic substrate make this a promising approach for applications in surface-sensitive spectroscopies. Translating this exfoliation method into vacuum could allow development of strategies for the preparation of 2D materials with controlled interfaces and tailored properties, which is the focus of our work.

The first strategy involves exfoliation on patterned Au/SiO_2 substrates, where a single flake spans regions of distinct substrate interaction [2]. This geometry allows direct comparison of substrate-induced effects, such as the role of stronger (Au) or weaker (SiO_2) screening, within the same 2D material. Initial experiments using graphene demonstrate successful transfer across both Au and SiO_2 regions, as confirmed by optical microscopy and atomic force microscopy.

The long-term goal is to extend these approaches toward vacuum-compatible preparation methods, such as the Kinetic *In situ* Single-layer Synthesis (KISS) technique [3], enabling polymer-free sample fabrication. This would allow direct investigation of clean 2D material interfaces using angle-resolved photoemission spectroscopy (ARPES) and X-ray photoelectron spectroscopy (XPS).

With these developments we aim to establish a versatile pathway from exfoliation to spectroscopic characterization of pristine 2D material interfaces, and ultimately provide a way to control the properties of 2D materials through interface engineering.

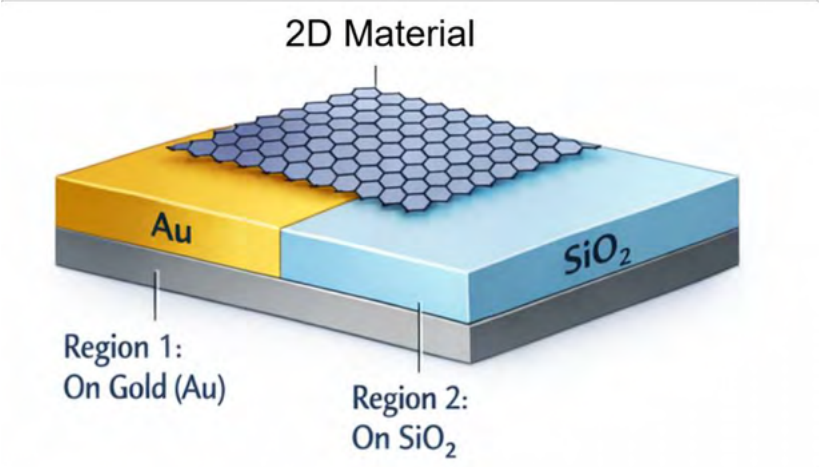

Figure 1. Schematic of a 2D material flake spanning both Au and SiO_2 regions.

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Electronic Structure of Multiferroic SnSe from Monolayer to Bulk

Dina Wilks,[1] Mahdi Ghorbani-Asl,[2] Thais Chagas,[1] Pedro H. R. Goncalves,[3] Marcin Rosmus,[4] Tomasz Sobol,[5] Alice Bremerich,[1] Edyta Beyer,[5] Babara Wolanin,[5] Jenny Schrage,[1] Jonas Daub,[1] Andres F. Santander-Syro,[4] Arkadi V. Krasheninnikov,[2] Carsten Busse[1]

1) Department Physik, Universität Siegen, Walter-Flex-Straße 3, 57072 Siegen
2) Institute of Ion Beam Physics and Materials Research Helmholtz-Zentrum Dresden-Rossendorf 01328 Dresden, Germany
3) Department of Physics, Universidade Federal de Minas Gerais, Av. Pres. Antonio Carlos, 6627 – Belo Horizonte, Brazil
4) Université Paris-Saclay, CNRS, Institut des Sciences Moléculaires d'Orsay, 91405, Orsay, France
5) SOLARIS National Synchrotron Radiation Centre, Jagiellonian University, 31-007 Krakow, Poland

For conventional ferroelectrics the critical temperature T_c quickly falls below technically feasible values for very thin films. This is not the case for two-dimensional (2D) materials. Theory predicts strong ferroelectricity for group IV monochalcogenides, whose individual layers are puckered sheets with a phosphorene-like structure that lack inversion symmetry. For SnSe, stable ferroelectricity of monolayer (ML) and thin films at room temperature has been demonstrated [1-3]. Moreover, SnSe thin films were shown to be ferroelastic [3]. Bulk SnSe, however, is not ferroelectric, due to its stacking which restores symmetry. Here, we provide the missing experimental determination of the band structure of ML SnSe and its evolution with increasing layer thickness.

We use angle-resolved photoemission spectroscopy (ARPES) to determine the valence band structure of SnSe ML, bilayer (BL) and six-layer (6L), investigate the influence of the substrate, and examine differences in stacking between few-layer films and the bulk. SnSe films are prepared by molecular beam epitaxy (MBE) using graphene on Ir(111) as an inert and weakly interacting substrate [**4**]. We observe a clear transformation of the band structure from ML to 6L and to the bulk: new bands emerge while others vanish. Density functional theory (DFT) calculations for freestanding SnSe corroborate these findings, albeit with a shift to lower binding energies. We attribute this shift to charge transfer between the SnSe layers and the substrate.

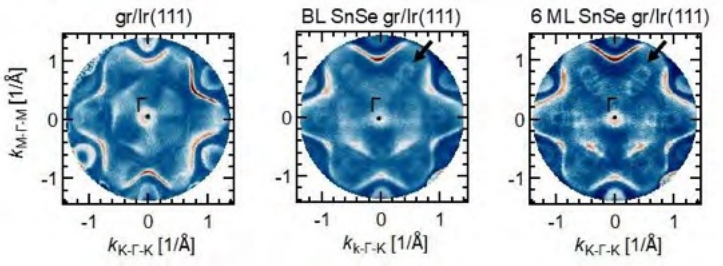

Figure 1: ARPES intensity maps a $\boldsymbol{E_b = -0.2}$ eV of gr/Ir(111), BL and six-layer SnSe on gr/Ir(111).

References

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Thermally driven α-β phase transition and alloy formation in SnSe/Au(111)

E. Tosi,[1] V. Villalobos-Vilda,[1] S. Jiménez-Fernández,[1] J. I. Martínez,[1] P. Lacovig,[2] S. Lizzit,[2] L. Sangabattula,[1] F. J. Fernández-Alonso,[1] I. Palacio,[1] M. F. López,[1] J. A. Martín-Gago,[1] C. Sánchez-Sánchez,[1]

1) Instituto de Ciencia de Materiales de Madrid (ICMM-CSIC), C/Sor Juana Inés de la Cruz 3, Madrid, Spain
2) Elettra-Sincrotrone Trieste S.C.p.A., AREA Science Park, S.S. 14 km 163.5, 34149 Trieste, Italy

Two-dimensional metal monochalcogenides grown epitaxially on crystalline substrates offer a versatile platform to explore phase stability, interface reactivity, and thermally activated transitions. In particular, SnSe on Au(111) exhibits multiple competing structural phases whose stabilization depends sensitively on growth and post-growth conditions. While previous studies have demonstrated selective preparation of α- and β-SnSe, the full thermally driven evolution of this epitaxial system remains largely unexplored. Here we present a comprehensive surface-science study of the temperature-induced transformation pathway of epitaxial SnSe on Au(111), revealing a sequential α-SnSe → β-SnSe → Au_2Sn evolution confined to the surface. Using real-time temperature programmed XPS, complemented by temperaturedependent LEED and STM, we resolve three distinct regimes: (i) desorption of α-SnSe multilayers, (ii) emergence and stabilization of β-SnSe monolayer as contact phase, and (iii) Se depletion accompanied by Sn incorporation into the Au(111) lattice, leading to the formation of a crystalline two-dimensional Au_2Sn surface alloy. Our results provide direct experimental insight into how thermal energy governs phase competition, dimensionality reduction, and chemical reactivity at a chalcogenide/metal interface. Beyond refining the static growth phase diagram of SnSe/Au(111), this work establishes a mechanistic framework for thermally driven transformations between epitaxial 2D materials and surface alloys, highlighting temperature as an effective control parameter for engineering functional low-dimensional phases on metal substrates.

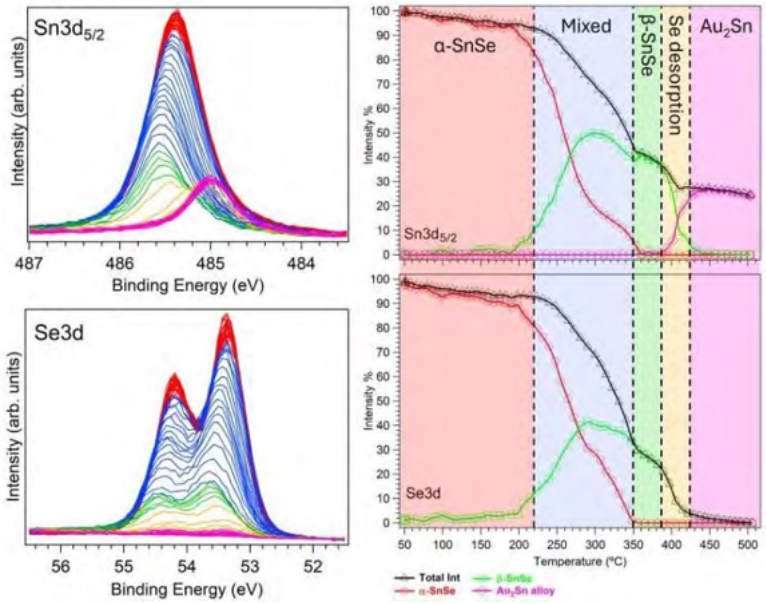

Figure 1: Temperature-programmed XPS of the α→β→alloy transition in SnSe/Au(111).

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Multifunctional Momentum Microscopy for 2D material research

Saumya Mukherjee[1], Marten Patt[1], Stefan Böttcher[1], Nils Weber[1], Timna Kühn[1], Matthias Escher[1]

1) SPECS Surface Nano Analysis GmbH, 13355 Berlin, Germany

Energy-filtered photoelectron microscopes have been used for various applications including work-function mapping, imaging XPS and in the last years more prominently for imaging the reciprocal space, i.e., momentum microscopy. A big advantage of momentum microscopy is that it projects the sample surface in real space as well as the angular distribution (ARPES) of the electrons. This allows us to study the electronic properties, including spin properties, of graphene and 2D materials on locally defined sample regions [1]. In combination with XPS light sources, complementary measurements like the chemical mapping of the surface become possible, which allows for a precise classification of 2D material heterostructures [2].

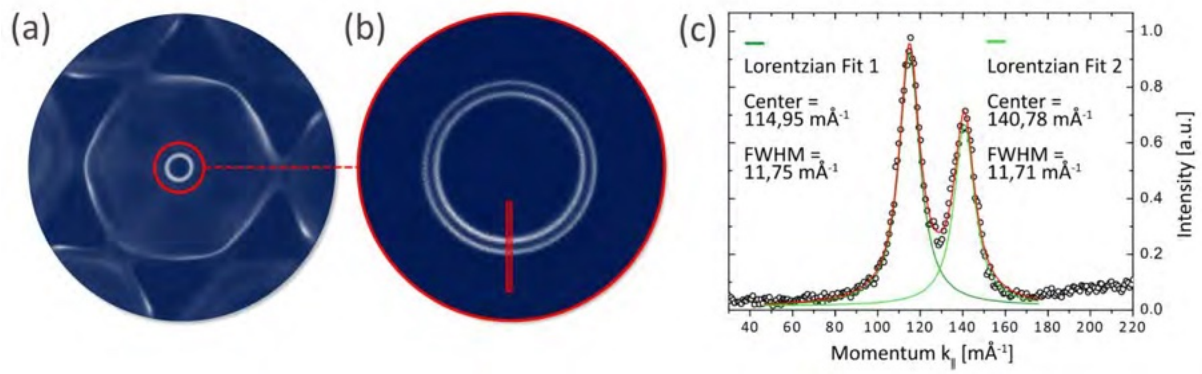

Figure 1: (a) Momentum Space Microscopy Image of a Au (111) single crystal at the Fermi level, showing more than one Brillouin zone. (b) Zoom onto the Rashba split surface state of Au (111). This image was taken at a sample stage temperature of 45 K. The instrumental energy resolution was evaluated to be < 24 meV by fitting the Fermi edge and subtracting the thermal broadening. The line profiles of the bands were fitted with Lorentzian peak functions. The natural broadening of the bands are significantly bigger than the Gaussian broadening of the instrumental resolution.

We designed a new microscopy system which combines the Focus NanoESCA [3] MARIS and TOF MARIS analyzers with the powerful light sources and system bases of SPECS. This system is modular and can be tailored to the analytic needs of the current field of research and upgraded later, when the research prospers. We establish Momentum Microscopy as a comprehensive tool for graphene and 2D material characterization, covering real-space imaging, band structure study, spin- and time-resolved analysis. We will demonstrate performance advancements and present a detailed overview of new developments, e.g. in the field of high-efficiency spin-resolved imaging [4].

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Strain it, sculpt it, cut it: Thermal scanning probe lithography in 2D materials research

TheofylaktopoulosV[1],UbezioA[1]

1) Heidelberg Instruments Nano

Thermal scanning probe lithography is a direct write lithography technique. It relies on a hot cantilever sublimating a thermal resist to define patterns with resolution below 15nm. It has found applications in nanoelectronics, plasmonics, nanofluidics and bio-surface research [1]. In the last few years, the number of publications in the field of 2D materials research has been growing. In this talk, we will go through the techniques to strain [2,3], cut [4] and sculpt [5] 2D materials.

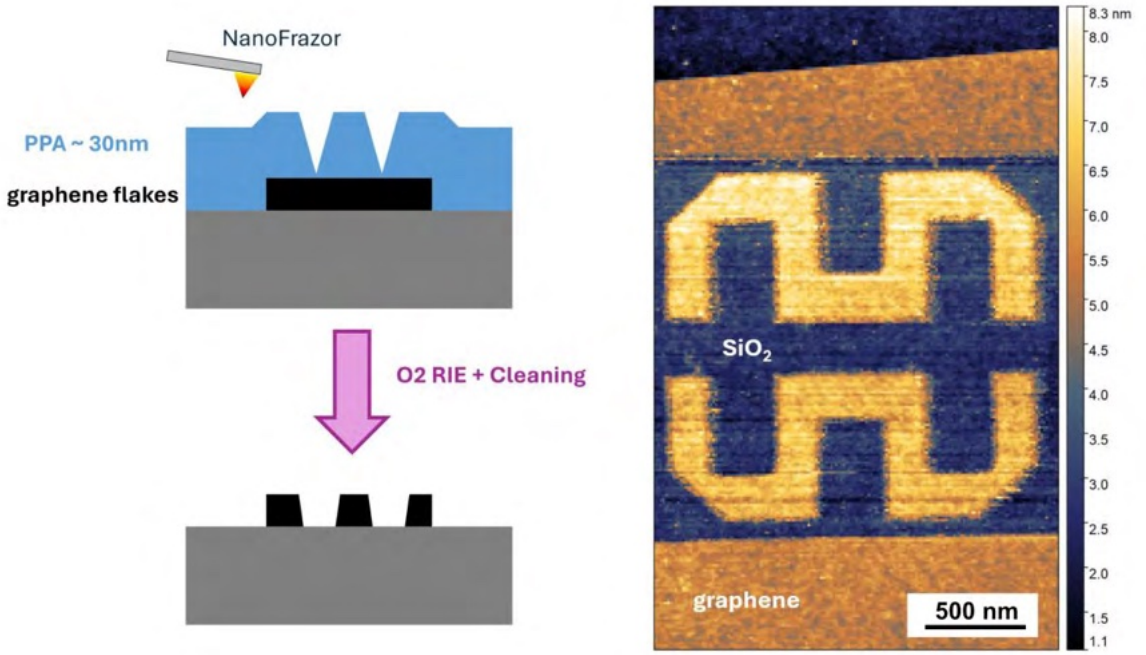

Figure 1: Etched graphene in the logo of Heidelberg Instruments using a one-layer polyphthalaldehyde (PPA) and O_2 reactive ion etching workflow.

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Probing electronic disorder in nanomaterials with coherent two-dimensional spectroscopy

T. Kawde[1], P. Trofimov[1], M. Russo[1], A. Trenczek[1], and H. Seiler[1]

1) Freie Universität Berlin, Germany

Static inhomogeneities and dynamical fluctuations are inherent to nanomaterials and understanding their impact on electronic properties is highly relevant for applications. Coherent spectroscopy two-dimensional (2D) is a powerful tool to separate static and dynamic sources of disorder. Here we introduce a 2D spectroscopy setup to investigate excitons and polaritons in van der Waals 2D materials and heterostructures, which are often only 10-20 μm in size and spatially heterogeneous. The 2D spectrometer is integrated with a confocal back focal plane imaging setup, featuring high magnification, spatial and angle resolution, while maintaining a time resolution of ~15 fs. We demonstrate the approach on an exfoliated WSe_2 monolayer, resolving A-exciton lineshape dynamics. The data reveal <100 fs homogeneous linewidth broadening, indicating that dynamical fluctuations of the exciton-energy proceed on the femtosecond timescale. These measurements provide insight into dephasing mechanisms such as excitation-induced dephasing, which set fundamental limits to coherent control and quantum-optical applications.

Charge and resonant energy transfer in hybrid organic-TMDs heterostructures

Š. Mandić[1,2], A. Senkić[3], N. Vujičić[1]

1) Centre for Advanced Laser Techniques, Institute of Physics, Bijenička cesta 46, 10 000 Zagreb, Croatia
2) Faculty of Physics, University of Rijeka, Ulica Radmile Matejčić 2, 51 000 Rijeka, Croatia
3) Institute of Physics, University of Münster, Wilhelm-Klemm str. 10, 48149 Münster, Germany

Organic–inorganic heterostructures (HS) represent a versatile platform for tailoring light–matter interactions by combining molecular semiconductors with two-dimensional materials. These hybrid systems enable tunable excitonic behavior, interfacial charge transfer, and band alignment control beyond what is achievable in the individual constituents [1].

In this work, we investigate the impact of a thin layer of metal-free phthalocyanine (H_2Pc) on the optical properties of the two-dimensional semiconductors MoS_2 and WS_2. The complementary optical, structural, and electrostatic measurements reveal that H_2Pc functionalization induces pronounced modifications in both excitonic emission and vibrational modes. We identify distinct charge– and energy-transfer pathways for different HS. In H_2Pc/MoS_2, electron transfer from MoS_2 to H_2Pc is dominant process, accompanied by molecular "defect healing," where H_2Pc passivates MoS_2 defect sites and improves material quality. In contrast, the H_2Pc/WS_2 heterostructure exhibits Förster resonance energy transfer, confirmed by dual-component emission and quenched WS_2 photoluminescence under resonant conditions. Raman analysis of the molecular vibrations further supports the differing interaction mechanisms. Our results demonstrate that the interaction between organic molecules and 2D materials is governed by subtle details of the electronic structure, defect landscape, and molecular dipole moments [2].

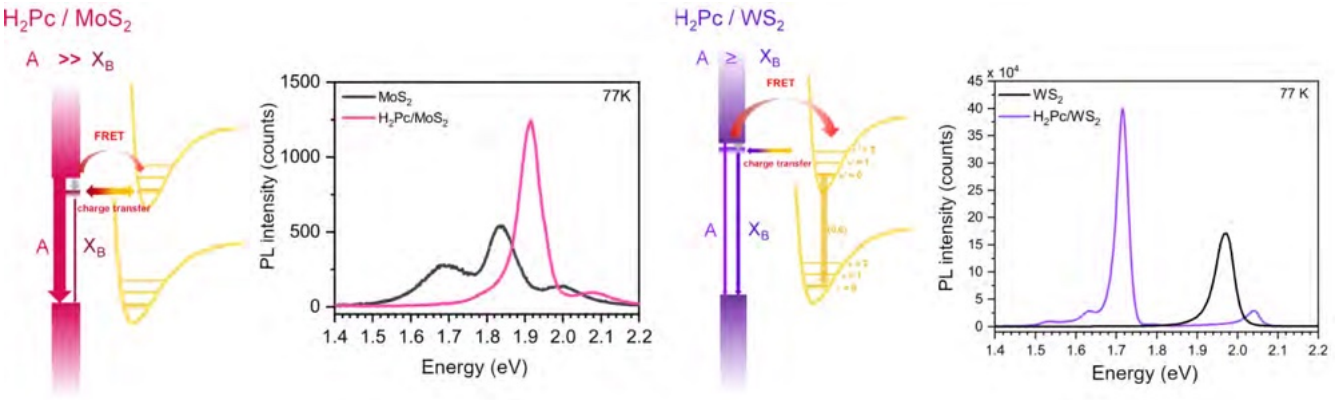

Figure 1: Charge transfer and Förster resonant energy transfer in H_2Pc/TMD heterostructures. Low-temperature (77 K) photoluminescence (PL) spectra of as-grown MoS_2 (grey) and H_2Pc/MoS_2 (pink), and of as-grown WS_2 (black) and WS_2/H_2Pc (violet) heterostructures

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Recent developments in epitaxially grown 2D magnets: From 2D-XY systems to high-Tc magnets driven by self-intercalation

Amilcar Bedoya-Pinto,[1]

1) Institute of Molecular Science, University of Valencia (Spain)

2)

In this talk, I will discuss how the bottom-up growth of van der Waals magnets by molecular beam epitaxy (MBE) promotes favorable conditions to stabilize particular magnetic behavior which has remained elusive on studies with exfoliated bulk crystal flakes – such as XY anisotropy and enhancement of magnetic exchange driven by self-intercalation.

First, I will focus on the successful van-der-Waals epitaxy of a $CrCl_3$ monolayer grown on Graphene/6HSiC(0001), whereby *in-situ* X-ray magnetic circular dichroism studies reveal intrinsic ferromagnetic order with easy-plane anisotropy and a 2D-XY magnetic universality class [1]. This constitutes the first realization of a Berezinskii-Kosterlitz-Thouless (BKT) transition in a two dimensional magnet, and further allows the stabilization of topological spin textures with in-plane winding, such as merons. The important role of the van der Waals substrate interaction and the underlying crystal symmetry to achieve this rather unsual magnetic behavior will be discussed, thereby highlighting routes on how to control the anisotropy of 2D magnets via growth and substrate engineering.

Further peculiarities of MBE-grown van der Waals magnets, such as an increase of the Curie Temperature driven by self-intercalation [2], will be shown in the prototypical high-Tc magnet Fe_5GeTe_2. The epitaxial films were prepared by molecular beam epitaxy on Al_2O_3 (0001) and their magnetic properties explored by XMCD, showing ferromagnetic ordering up to 375 K. A sizable Fe occupation within the van der Waals gaps was determined by high-precision x-ray diffraction analysis and transmission electron microscopy (TEM). Supported by first-principles calculations, we infer that the higher magnetic ordering temperature results from an increased exchange interaction among the Fe_5GeTe_2 layers mediated by Fe within the vdW gaps. Our findings establish self-intercalation during epitaxial growth as an efficient mechanism to achieve high-temperature magnetism in a broad class of van der Waals materials.

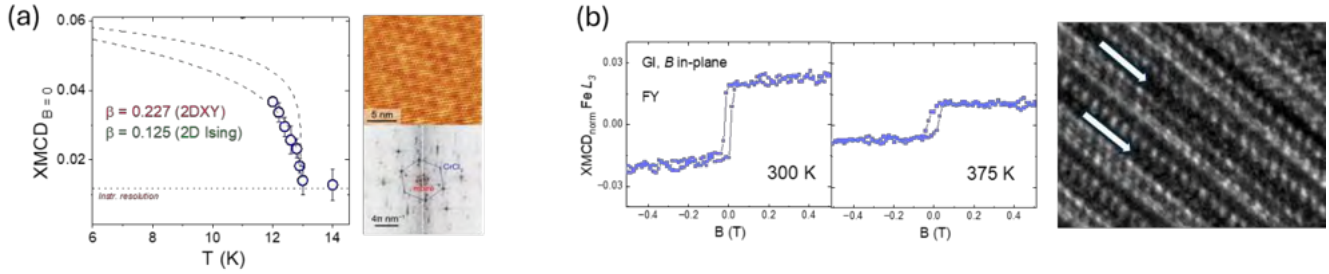

Figure 1: (a) Critical exponent fits of the magnetic moment at remanence (XMCD, B=0) of a monolayer $CrCl_3$ showing 2DXY scaling, along with a scanning tunneling microscopy image showing a characteristic moire pattern of $CrCl_3$ on graphene. (b) Ferromagnetic hysteresis of the XMCD signal in epitaxial Fe_5GeTe_2 showing finite remanence at 375K. Fe-atoms within the vdW gaps are visualized in transmission electron microscopy (TEM) imaging.

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Evidence of multiferroicity in monolayer $NiBr_2$

A. Karjasilta,[1] A. Cahlik,[1] A. Fumega,[1] A. Mishra,[1] R. Drost,[1] M. Amini,[1] J. Arshad,[1] B. Arslan,[1] J. Lado,[1] and P. Liljeroth[1]

1) Department of Applied Physics, Aalto University, PO Box 15100, 00076 Aalto, Finland

Multiferroic materials exhibit more than one primary ferroic order, such as ferromagnetism and ferroelectricity. Progress in two-dimensional (2D) materials has proven monolayer NiI_2 to be the first multiferroic material at single-layer limit[1]. Here we present experimental evidence of multiferroicity in monolayer $NiBr_2$, another transition metal dihalide (TMDH), by using scanning tunneling microscopy (STM) and scanning tunneling spectroscopy (STS). These techniques have demonstrated the capacity to investigate monolayer multiferroicity at atomic scale[2]. Surprisingly, we observe two different stripe periodicities, ~14 Å and ~28 Å. Furthermore, we are able to switch between these by altering our setpoint or applied external magnetic field. These findings are important for further understanding of multiferroicity down to monolayer limit.

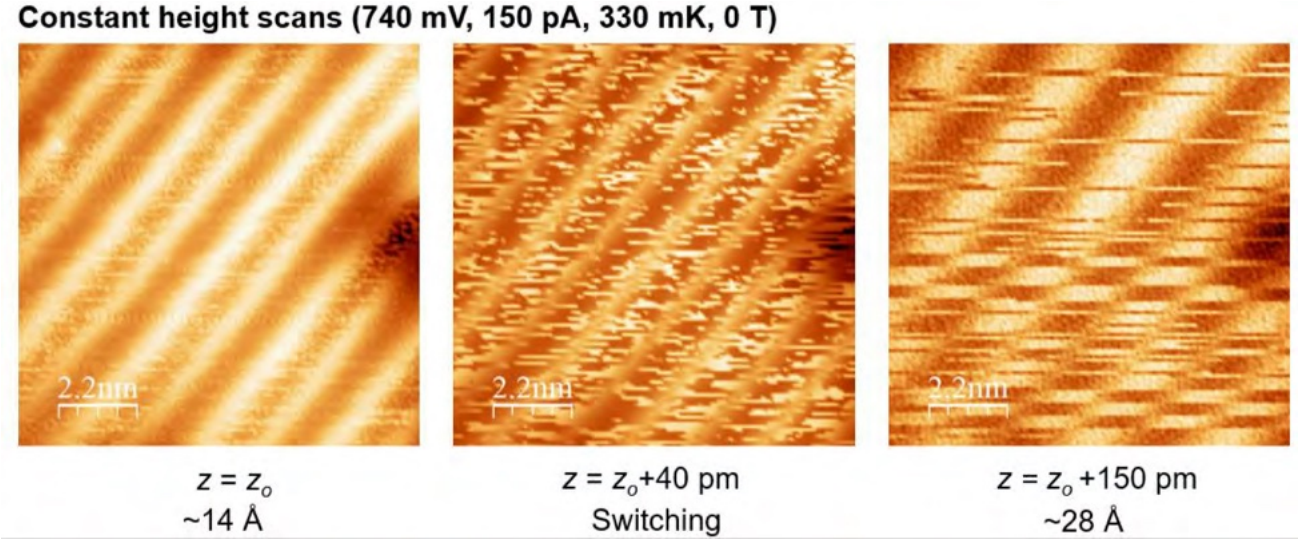

Figure 1: Change of stripe periodicity when the tip-sample distance increases.

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Ferroelectric domain boundaries as internal quantum wells in van der Waals TMDs

Li, X.[1,2], McHugh, J. G.[1,2], Soltero, I.[1,2], Falko, V.[1,2]

1) Department of Physics and Astronomy, University of Manchester, Oxford Road, Manchester, M13 9PL, United Kingdom

2) National Graphene Institute, University of Manchester, Booth St. E., Manchester, M13 9PL, United Kingdom

Ferroelectricity emerging in stacked two-dimensional (2D) transition metal dichalcogenides (TMDs) provides an intrinsic route to engineer electronic properties in layered materials.[1,2] In rhombohedral (3R) TMDs, the lack of inversion symmetry leads to pronounced interlayer charge redistribution, giving rise to robust out-of-plane ferroelectric polarization and strong internal electric fields.[3] These built-in fields naturally confine electrons and holes into atomically thin quantum wells at interfaces between domains of opposite polarization, known as mirror twin boundaries (mTBs).[4,5] We combine first-principles density functional theory (DFT) with a self-consistent Thomas-Fermi approach to establish a predictive framework for polarization-driven quantum confinement at ferroelectric twin boundaries in van der Waals TMDs, enabling systematic evaluation of carrier accumulation, confinement stability, and external tunability across a broad materials space (Figure 1). This work establishes ferroelectric mTBs as a programmable internal-interface platform for hybrid integration, enabling built-in fields to define and tune quantum-confined channels relevant to nanoscale optoelectronic, photonic, and quantum device architectures, while reducing reliance on external gating and complex heterostructures.

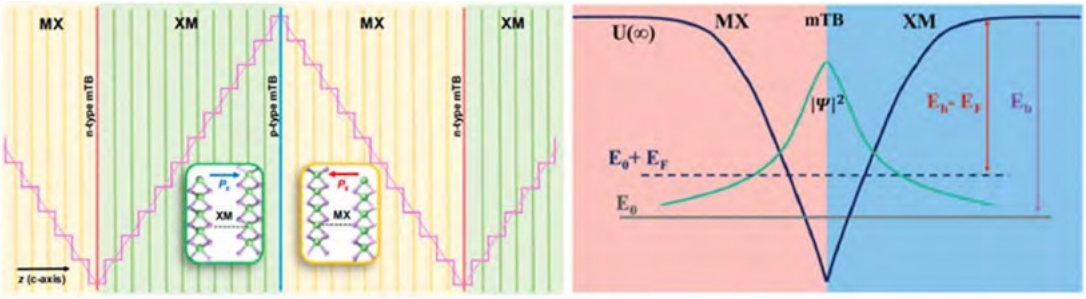

Figure 1: (Left) Mirror twin boundaries in ferroelectric TMDs. Schematic of mirror twin boundaries separating adjacent ferroelectric domains in 3R-TMDs (with MX- and XM-stacking). (Right) Schematic illustration of the electrostatic potential profile across a mTBs, and the green curve displays the probability density ($|\Psi(z)|^2$) of accumulated carriers. The black curve is the potential profile in triangular well.

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POSTER ABSTRACTS

MicroARPES benchmark of exfoliated hBN and a moiré-induced minigap with replicas on monolayer hBN in twisted graphene/hBN

Zhihao Jiang,1† Gianmarco Gatti,1† Gesa-R Siemann,1 Charlotte Sanders,2 Anders S Mortensen,1 Hippolyte R. Bourel,1 Alfred J. H. Jones,1 Matthew D. Watson,3 Timur K. Kim,3 Kenji Watanabe,4 Takashi Taniguchi,5 Yong P. Chen,1,6 Jill A. Miwa,1 Søren Ulstrup,1 and Philip Hofmann*1

1) Department of Physics and Astronomy, Interdisciplinary Nanoscience Center, Aarhus University, 8000 Aarhus C, Denmark

2) Central Laser Facility, STFC Rutherford Appleton Laboratory, OX11 0QX Harwell, United Kingdom

3) Diamond Light Source, Division of Science, Didcot, OX110DE UK

4) Research Center for Electronic and Optical Materials, National Institute for Materials Science, 1-1 Namiki, Tsukuba 305-0044, Japan

5) Research Center for Materials Nanoarchitectonics, National Institute for Materials Science, 1-1 Namiki, Tsukuba 305-0044, Japan

6) WPI Advanced Institute for Materials Research (AIMR), Tohoku University, Sendai 980-8577, Japan

Hexagonal boron nitride (hBN) is the ubiquitous dielectric, encapsulation, and tunneling barrier for graphene and van der Waals devices, yet a systematic experimental benchmark of its electronic structure as a function of thickness remains scarce[1-3]. Here we establish a comprehensive micro-ARPES dataset of mechanically exfoliated hBN spanning monolayer, bilayer, trilayer, four-layer, thin flakes, and bulk crystals, measured with consistent energy calibration and analysis workflows. By comparing valence-band dispersions across the Brillouin zone, we extract thickness-dependent trends in the valence-band maximum, characteristic band splittings/broadening, and the crossover from a two-dimensional limit to bulk-like behavior driven by interlayer coupling. Building on this reference, we present a focused case study of a twisted graphene/monolayer-hBN heterostructure at a fixed relative orientation. Remarkably, we directly observe a gap opening on an hBN-derived band accompanied by clear replica features, consistent with moiré-driven band reconstruction via interlayer coupling and superlattice (umklapp) scattering. This combined benchmark-and-case-study approach links pristine hBN thickness evolution to moiré-induced spectral fingerprints on hBN itself, providing an experimental foundation for band alignment and for disentangling graphene- versus hBN-originated replicas and minigaps in graphene/hBN devices.

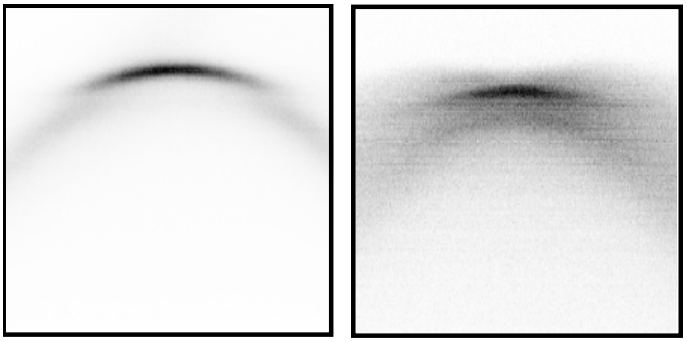

Figure 1: Electronic structure of K-point of monolayer hBN with a gap (left) and bulk hBN (right).

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Epitaxial Strain Stabilizes the Ferroelectric SnSe Phase in the Monolayer Limit

Dina Wilks,[1] Vedran Vonk,[2] Paulus Aleksa,[1] Simon Chung,[2] Simon Geile,[2] Alice Bremerich,[1]
Thais Chagas,[1] Dimitri V. Novikov,[3] Peter Modregger,[1] Andreas Stierle,[2,4] Carsten Busse[1]

1) Department Physik, Universität Siegen, Walter-Flex-Straße 3, 57072 Siegen
2) Centre for X-ray and Nano Science CXNS, Deutsches Elektronen-Synchrotron DESY, Notkestr. 85, 22607 Hamburg, Germany
3) Photon Science, Deutsches Electronen-Synchrotron DESY, Deutsches Elektronen-Synchrotron DESY, Notkestr. 85, Hamburg, 22607, Germany
4) Department of Physics, University of Hamburg, Notkestr. 9-11, 22607 Hamburg, Germany

Two-dimensional orthorhombic SnSe is predicted to exhibit robust in-plane ferroelectricity down to the monolayer limit, in contrast to conventional thin-film ferroelectrics. Previous studies have reported ferroelectric behavior in SnSe on graphitized 6H-SiC(0001) using scanning tunneling spectroscopy [1], indicating a phase transition in the temperature range between 380 and 400 K. However, a direct crystallographic determination of this phase transition is still lacking.

To investigate the ferroelectric-to-paraelectric phase transition at the crystallographic level, mono- and few-layer SnSe films were grown on graphene/Ir(111) [2] by molecular beam epitaxy (MBE) under ultra-high vacuum conditions and studied using surface X-ray diffraction (SXRD). Temperature-dependent measurements up to 550 K show no phase transition for mono- and bilayer SnSe. Structurally, both mono- and bilayers exhibit a single phase with three distinct orientations relative to the graphene substrate. The zigzag direction of SnSe aligns with the armchair direction of graphene, and the lattice parameter b matches the periodicity of the graphene's armchair direction $\left(b = \sqrt{3}\, a_{\mathrm{gr}} \right)$. For six layers, the lattice parameters are closer to the bulk values and up to desorption temperature we observe a similar behaviour as in the bulk. These findings suggest a stabilization of the ferroelectric phase of mono- and bilayer SnSe induced by strain.

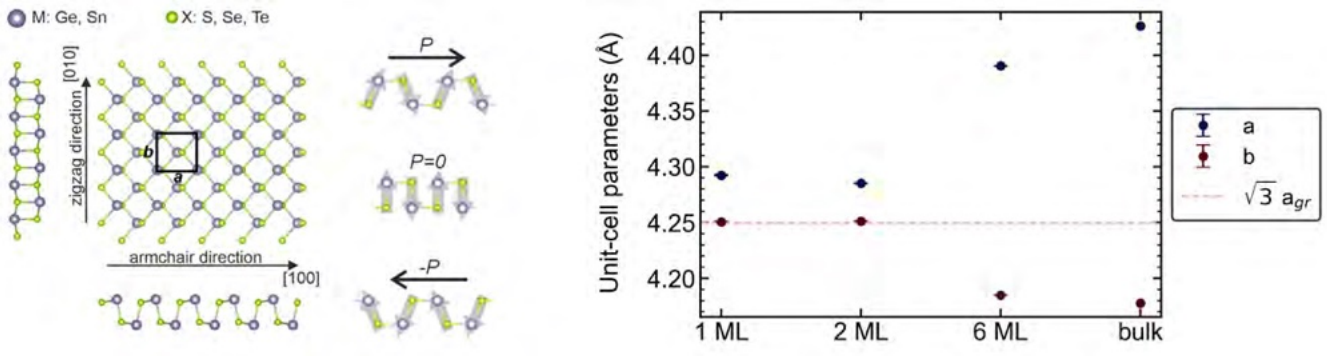

Figure 1: Left: Top and side view of SnSe, along with schematic side views illustrating the polarization in the ferroelectric phase ($\boldsymbol{P \neq 0}$) and the symmetric paraelectric phase ($\boldsymbol{P = 0}$). Right: In-plane unit-cell parameters depending on layer thickness as well as the bulk values [3].

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Emergence of flat band via strong Moiré potential in Honeycomb BeO-based system

Sungsoo Hahn,[1] Jacek Osiecki,[1] Craig Polley,[1] Mats Leandersson,[1] Balasubramanian Thiagarajan, [1]

1) MAX IV Laboratory, Lund University, 221 00 Lund, Sweden

Monolayer honeycomb BeO (h-BeO) is a 2D material with a wide band gap (~6 eV) arising from strong ionic Be–O bonding. The ionic character of this bond is expected to generate stronger local electric field, making h-BeO a promising building block for Moiré interfaces distinct from graphene and hBN. Here, we investigate the Moiré-engineered band structure of h-BeO/BeO(0001) interface using angle-resolved photoemission spectroscopy (ARPES). Monolayer h-BeO was successfully grown by annealing Be(0001) surface under an oxygen atmosphere.

ARPES measurement reveals not only the honeycomb-characteristic band structure of BeO, but also the emergence of a Moiré-potential-induced flat band derived from Be surface state. This result not only provides an h-BeO growth method, bult also demonstrates that h-BeO can serve as an effective building block for Moiré-engineering.

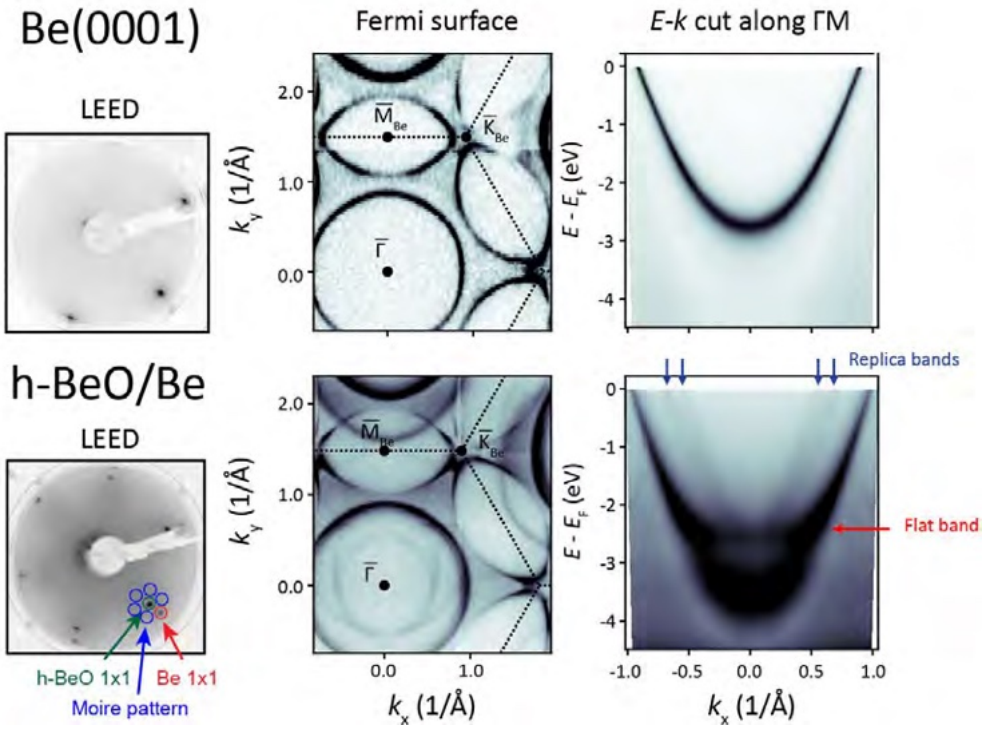

Figure 1: LEED and ARPES result of Be(0001) and h-BeO/Be.

From embedded nuclei to extended islands: key processes in epitaxial growth of tantalum sulfide on Au(111)

Catherine Grover[1], Alice Bremerich[1], Dina Wilks[1], Kai Mehlich[1], Abdus Samad[2], Udo Schwingenschlögl[2], Carsten Busse[1], and Thais Chagas[1]

1) Department Physik, Universität Siegen, 57068 Siegen, Germany
2) Physical Science and Engineering Division, King Abdullah University of Science and Technology, 23955-6900 Thuwal, Saudi Arabia

The atomic-scale pathways that connect the nuclei to extended two-dimensional materials remain poorly understood, despite their critical role in determining the structure and phase of epitaxial layers. Here, we combine scanning tunneling microscopy and density functional theory to investigate the epitaxial growth of tantalum sulfides on Au(111). Growth begins with a well-defined sequence from embedded TaS_3 nuclei that evolve into larger embedded Ta_3S_6 islands before giving rise to adsorbed TaS islands. Height measurements identify the critical size at which these structures emerge from the substrate, marking the onset of epitaxial growth (Fig. 1). By tuning the sulfur chemical potential, we further demonstrate control over island morphology and edge termination. Our results provide a unified picture of the initial growth stages of tantalum sulfides. We propose that in general, embedded nuclei play a key role in governing the early growth pathways of two-dimensional transition-metal chalcogenides on metal substrates.

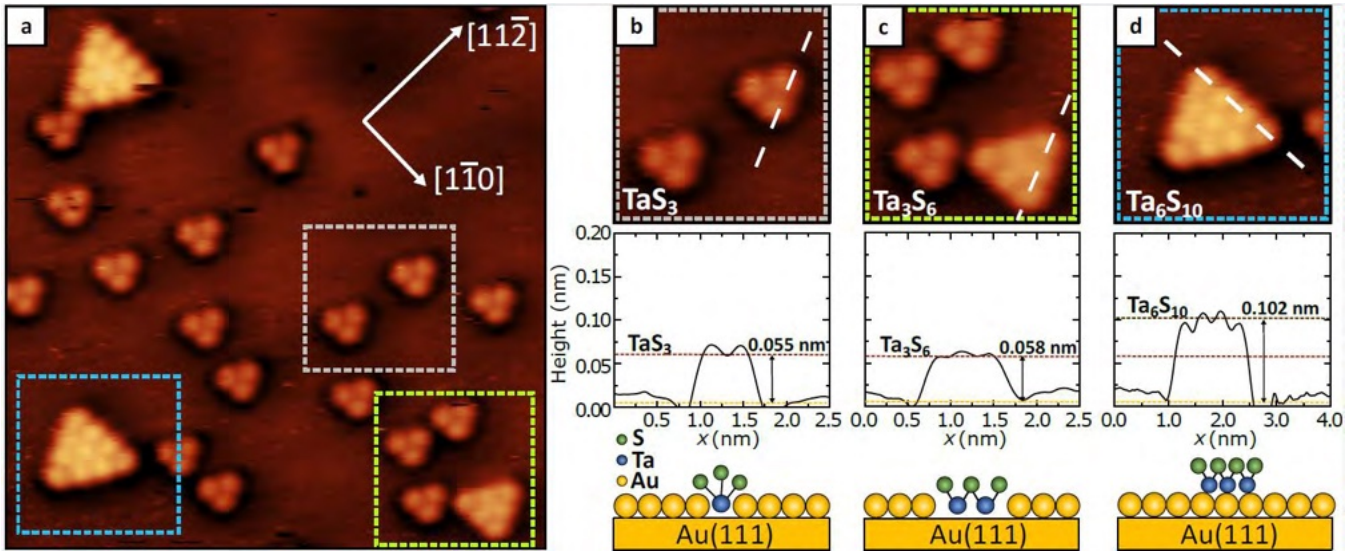

Figure 1: STM images showing (a) a large area containing TaS_3 nuclei, a Ta_3S_6 island, and two Ta_6S_{10} islands. The magnified images dashed outlines color-matched to those in (a) show (b) embedded TaS_3, (c) embedded Ta_3S_6, and (d) adsorbed Ta_6S_{10}. The corresponding height profiles (along dashed white lines shown in (a)) and schematics are shown for each structure in the middle and bottom panels, respectively. In the profiles, the gold dashed line corresponds to the Au(111) substrate, red to the TaS_3 and Ta_3S_6 structures, and brown to the Ta_6S_{10}. Image parameters: (a–d) $V = -0.34$ V and $I = 5.40$ nA. Image sizes: (a) 12.0 nm × 12.0 nm, (b) 3.5 nm × 3.5 nm, (c) 3.5 nm × 3.5 nm, and (d) 4.0 nm × 4.0 nm.

Proximity-Induced Superconductivity and Topological Phases in Pb/$BiSbTeSe_2$ Heterostructure

Richard Balog, Liv Hornekaer, Yong P. Chen

Department of Physics and Astronomy, Aarhus University, Denmark

The interface between topological insulators (TIs) and s-wave superconductors provides a robust platform for realizing topological superconductivity and Majorana zero modes [1]. In this study, we investigate the proximity effect in heterostructure of the bulk-insulating topological insulator $BiSbTeSe_2$ (BSTS) and superconducting Lead (Pb).

Using Scanning Tunneling Microscopy (STM) at a base temperature of 0.3 K, we characterize the evolution of the superconducting gap across the Pb/BSTS interface. Our spatially resolved spectroscopic measurements indicate a proximity-induced gap within the BSTS surface state. To further probe the nature of the induced order parameter and search for signatures of topological superconductivity, we examine the induced SC gap evolution inside an accidental antidot structure under high magnetic fields.

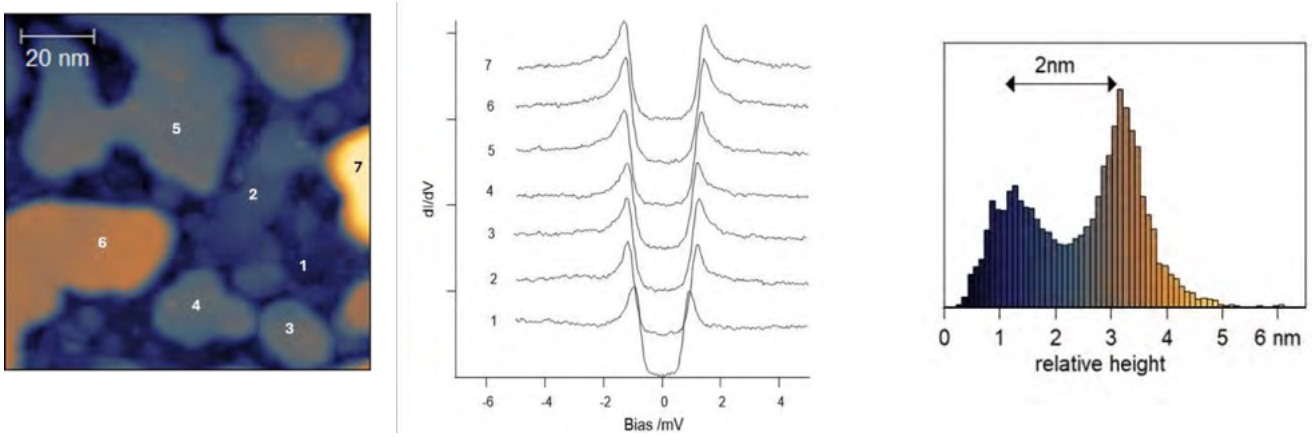

Figure 1: Left) Topographic STM image of Pb islands on cleaved BSTS; numbered sites denote local spectroscopy positions across varying thicknesses. Center) Thickness-dependent evolution of the superconducting gap, scaling from **0.9 meV** (thin regions) to **1.3 meV** (bulk-like islands). Right) Histogram of large area image (not shown), highlighting the typical height variation of investigated Pb islands.

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Crystallite Orientation and Lateral Material Distribution in TMD Thin Film Studied by Laboratory GIWAXS

Pribusova SlusnaL,[1] VegsoK,[2,3] NádaždyP,[1,2] KrajcovicovaTE,[1] SojkovaM,[1] JergelM,[2] SiffalovicP,[2,3] HulmanM,[1]

1) *Institute of Electrical Engineering, Slovak Academy of Sciences, Dúbravská cesta 9, 845 04 Bratislava, Slovakia*
2) *Institute of Physics, Slovak Academy of Sciences, Dúbravská cesta 9, 845 11 Bratislava, Slovakia*
3) *Centre for advanced materials application (CEMEA), Slovak Academy of Sciences, Dúbravská cesta 5807/9, 845 11 Bratislava, Slovakia*

Chemical vapor deposition (CVD) is widely used technique to prepare transition metal dichalcogenide (TMD) thin films, where parameters such as precursors, gas flow, substrate type, and thermal profiles influence the resulting crystalline orientation.
This study reports a laboratory-based method using Grazing-Incidence Wide-Angle X-ray Scattering (GIWAXS) to measure pole figures and reveal the texture and spatial distribution of TMD domain in thin films.
Hexagonal-phase $PtTe_2$ layers were synthesized by first depositing 4 nm platinum films onto c-plane sapphire substrates via magnetron sputtering at 600 °C. The films underwent tellurization in a CVD chamber at 650 °C for 30 minutes under a 5% H_2/95% Ar gas flow, using high-purity tellurium powder. Rapid cooling to room temperature ensured the formation of a pure hexagonal phase, confirmed by Raman spectroscopy through the characteristic E_g (110 cm^{-1}) and A_{1g} (160 cm^{-1}) modes. X-ray reflectivity (XRR) analysis verified a film thickness of 14.2 ± 0.5 nm with a low roughness of 1.8 ± 0.3 nm. Furthermore, the application of GIWAXS tomography in grazing incidence mode allowed for the spatial mapping of crystalline domains. This combination of pole figure measurements and tomography enables advanced laboratory-scale structural analysis of TMD films that was previously only possible on synchrotron beamlines.

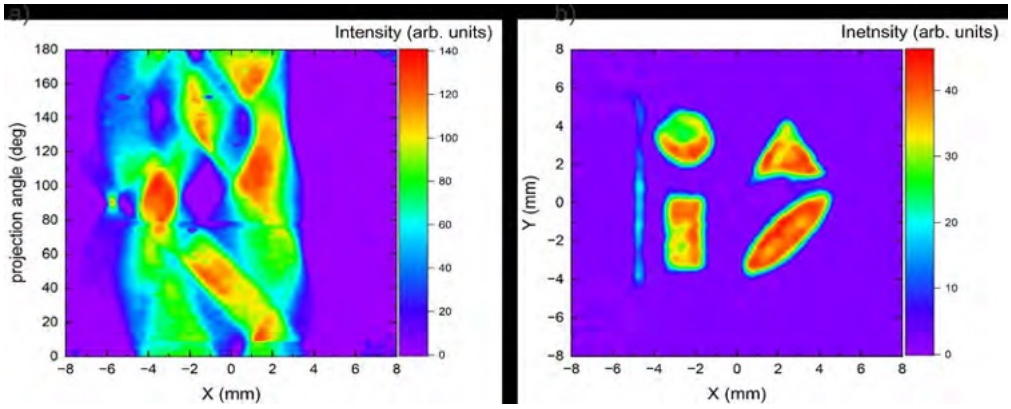

Figure 1: The experimental sinogram of the objects patterned in $PtTe_2$ film (left) b) the reconstructed image of the objects based on the filtered back-projection algorithm (right)

Aknowledgment
Authors are greatful to APVV-20-0111, APVV-23-0564, and APVV-24-0321, Danube Strategy 2024 project DS-FR-24-0059, Next Generation EU through the Recovery and Resilience Plan for Slovakia under the project No. 09I01-03-V04-00001 and 09I01-03-V04-00002.

Probing Optical Properties of Ultrathin TMD Films through Fabry–Perot Interference

Martin Hulman,[1] Lenka Pribusová Slušná, [1] Michaela Sojková, [1] Timea Krajčovičová, [1] Igor Píš [1]

1) Institute of Electrical Engineering, Slovak Academy of Sciences, Bratislava, Slovakia

Transition-metal dichalcogenides (TMDs) exhibit diverse electronic behaviours ranging from semiconducting to semimetallic. Optical spectroscopy provides an effective means of distinguishing materials with different electronic structures. Although optical spectra are often reported in the visible range, measurements in the infrared and far-infrared remain scarce.

We present optical measurements of selected TMD thin films across these spectral regions. Because the standard Kramers–Kronig approach cannot be directly applied to thin films on substrates, we employ an alternative method that monitors high-resolution variations in interference fringes within a Fabry–Perot resonator formed by the substrate, with the film acting as a perturbation.

For ultrathin layers of the order of 5–15 nm, the direct optical contribution of the TMD layer is very weak, and standard methods for extracting optical constants are laborious. Instead, we analyse changes in the amplitude and phase shift of the reflectivity oscillations, which arise from interference between light waves reflected from the substrate surfaces. These changes are extremely sensitive to the complex refractive index of the thin layer deposited on the substrate. By comparing measurements obtained by illuminating the sample from the front and back, one can quantitatively infer the transport properties of the thin layer. The difference between these two measurements directly reflects the thin film's optical conductivity. The ultimate goal is to determine the frequency-dependent optical conductivity. Differences among 2D materials and their possible relation to the band structure will be discussed.

Support from the project APVV-23-0564 is acknowledged.

Ultra-low energy ion irradiation of few-layer MoS_2: defect production and intercalation

Rabia Nawaz[1], Patrick James[1], Barbara Maria Mayer[2], Kenichiro Mizohata[1], Alvaro Lopez Cazalilla[3], E. Harriet Åhlgren[1,4,2]

1) Department of Physics, University of Helsinki, 00560 Helsinki, Finland.
2) Department of Physics and Astronomy, University of Uppsala, Uppsala SE-751 20, Sweden.
3) Barcelona Supercomputing Center, Plac¸a Eusebi G ¨uell 1-3, 08034, Barcelona, Spain
4) Faculty of Physics, University of Vienna, 1090 Vienna, Austria

Two-dimensional 2D materials such as molybdenum disulfide MoS_2 and other transition metal dichalcogenides have attracted strong interest due to their unique electronic, optical, and mechanical properties [1]. These materials show great potential for applications in electronics, optoelectronics, catalysis, and energy storage. Ion implantation is a powerful approach for modifying 2D materials by introducing controlled defects and dopants [2]. However, most studies focus on high-energy ions, while the effects of ultra-low-energy ion implantation on MoS_2 are still not well understood.

In this work, the effects of ultra-low-energy argon (Ar) and xenon (Xe) ion implantation on MoS_2 are studied using scanning transmission electron microscopy, Raman spectroscopy, and molecular dynamics simulations. Mechanically exfoliated MoS_2 samples were irradiated with the KIIA ion accelerator at the University of Helsinki at doses of 1x10^14 to 1x10^15 ions/cm^2 and ion energies of 15 to 200 eV. Structural analysis shows defect formation, while simulations reveal the onset of defect generation around 35 to 40 eV and ion trapping between MoS_2 layers at higher energies.

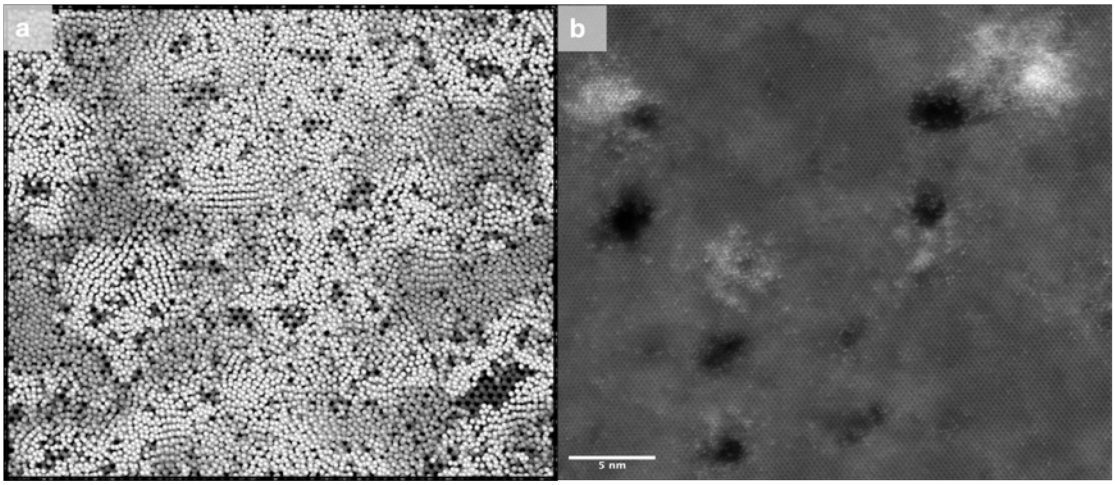

Figure 1: (a) Molecular dynamics simulation snapshot of Xe implantation into MoS_2 at an ion energy of 50 eV. (b) HAADF-STEM image of MoS_2 irradiated with Xe ions at 50 eV and a dose of 5×10^{14} ions cm^{-2}.

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Growth induced strain engineering in MoS_2 on graphene/Ir(332)

Karmen Kapustić,[1] Cosme González Ayani,[1] Fabián Calleja[2], Amadeo L. Vázquez de Parga[2], Iva Šrut Rakić[1]

1) Centre for Advanced Laser Techniques, Institute of Physics, Zagreb, Croatia
2) Instituto Madrileño de Estudios Avanzados IMDEA Nanociencia, Madrid, Spain

Strain plays an important role in tuning the properties of two-dimensional (2D) materials by modifying their electronic and mechanical behavior.[1] However, optical and transport measurements used to study these effects are inherently averaging techniques and therefore cannot resolve strain-induced phenomena at the nanoscale. Scanning tunneling microscopy (STM) and spectroscopy (STS) are excellent tools for investigating strain effects locally, as they provide direct access to structural and electronic properties.

Here, we introduce a novel approach for systematically inducing and probing strain in 2D materials at the nanoscale. As a model system, we synthesized monolayer MoS_2 on a pre-patterned substrate, graphene-covered Ir(332), consisting of two distinct facets: terraces and step bunches, using molecular beam epitaxy (MBE) under ultra-high vacuum (UHV) conditions. In our samples, monolayer MoS_2 islands bend over substrate step edges, resulting in the formation of uniaxial strain.

To obtain optimal samples for investigation, we performed a growth study and found that post-annealing temperature strongly influences the size and shape of MoS_2 islands. Higher temperatures yielded islands with more well-defined metallic edges and larger surface areas, which are beneficial for STS measurements. STS measurements performed at 77 K reveal variations in electronic structure that correlate with specific features of topography, as illustrated by the line STS map in Figure 1B, taken along the dashed line indicated in Figure 1A. We observe a non-rigid band shift on the step bunches vs. terraces and a band bending in the intermediate areas. A small modulation in the band-gap size is also observed, likely arising from local strain effects.

This work demonstrates a successful bottom-up approach for structurally modifying and straining MoS_2, providing a platform for nanoscale studies of strain-induced electronic and structural modifications.

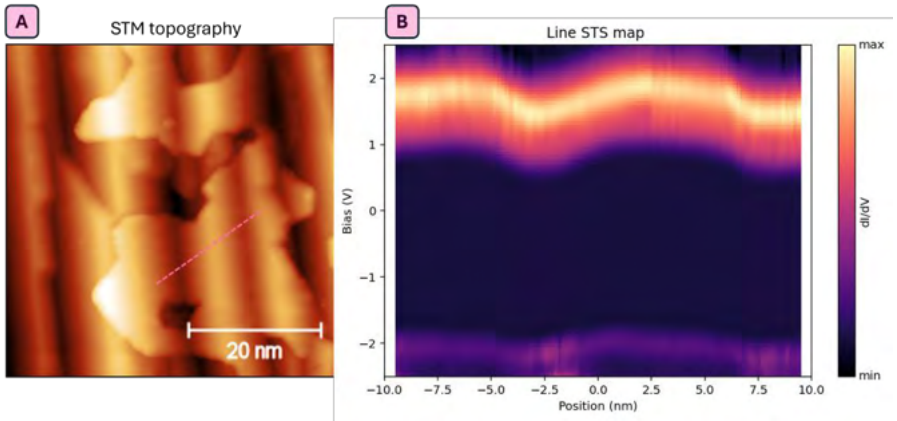

Figure 1: (A) Topography of the sample. The pink dashed line indicates where the line STS map in (B) was acquired at 77 K, showing local variations in the electronic structure that correlate with the topography.

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Emergent Nanoscale Phenomena in van der Waals MPX_3 Materials

Iva Šrut Rakić,[1] Lucija Malkoč,[1] Elena Voloshina,[2] Yuriy Dedkov,[1]

1) Centre for Advanced Laser Techniques, Institute of Physics, Zagreb, Croatia
2) Ruđer Bošković Institute, Zagreb, Croatia

Quasi-two-dimensional (quasi-2D) van der Waals (vdW) materials have emerged as fertile ground for the exploration of exotic optic, electronic and magnetic phenomena driven by reduced dimensionality, strong correlations and light–matter interactions, anisotropic dielectric response and variable interlayer bonding. Layered transition metal phosphorus trichalcogenides (MPX_3) form a versatile family of van der Waals antiferromagnets spanning a wide range of electronic band gaps, magnetic anisotropies, and spin–lattice coupling strengths, making them an attractive yet largely unexplored platform especially for polaritonic and strain-driven phenomena.[1]

Here we utilize an advanced atomic force microscopy (AFM) – based techniques to study polaritonic and solitonic phenomena in specific MPX_3 compounds, including $FePS_3$, $FePSe_3$, $CoPS_3$, and $MnPS_3$. Using scattering-type scanning near-field optical microscopy (s-SNOM), we find signatures of propagating polaritonic modes in these materials, constituting, to our knowledge, the first experimental observation of polaritons in the MPX_3 family. The measured interference fringes reveal guided optical modes in the visible spectral range, with propagation characteristics that vary across materials with different band gaps and dielectric response. In parallel, AFM, Kelvin probe force microscopy (KPFM), and conductive AFM (C-AFM) measurements reveal extended, line-like electronic and electrostatic features consistent with topological and structural soliton-like features at step edges induced by strain or stacking variations.

Our combined optical and scanning probe approach demonstrates how light–matter coupling and nanoscale electronic order intertwine in MPX_3 materials, providing a platform for studying hybrid quasiparticles and solitonic excitations in correlated two-dimensional magnets.

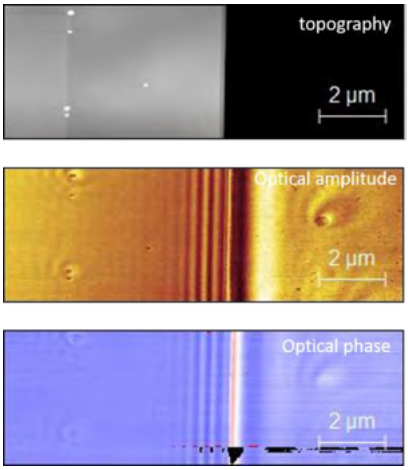

Figure 1: sSNOM measurements on $FePS_3$ on gold using a 633 nm excitation.

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Phase transition induced by dilute tungsten doping in CVD-grown MoS_2 bilayers

A. Senkić,[1] R. Keneipp,[2] P. Ivatović,[3] N. Pradeep,[2] V. Meunier,[4] M. Drndić,[2] N. Vujičić,[1] M. Kralj[1]

1) Centre for Advanced Laser Techniques, Institute of Physics, 10000 Zagreb, Croatia
2) Department of Physics and Astronomy, University of Pennsylvania, Philadelphia, PA, 19104, USA
3) Physics Department, Faculty of Natural Sciences, 10000 Zagreb, Croatia
4) Department of Engineering Science and Mechanics, Penn State University, University Park, PA, USA

Controlling the crystal phase and stacking order of two-dimensional (2D) transition metal dichalcogenides (TMDs) is essential for tailoring their optical, vibrational, and electronic properties. While phase transitions in monolayer TMDs and semiconductor-to-metal conversions have been extensively investigated, structural transitions between semiconducting polytypes–particularly in bilayer (2L) systems–remain comparatively underexplored. In bilayers, subtle changes in stacking symmetry can strongly modify inversion symmetry, interlayer coupling, and nonlinear optical responses, offering an additional degree of freedom for materials engineering. Here, we demonstrate a dilute tungsten (W) doping-induced phase transition from non-centrosymmetric AA stacking to centrosymmetric AB′ stacking in CVD-grown 2L MoS_2. By systematically increasing the W concentration, we observe a clear evolution of structural and optical signatures associated with the stacking transition. Polarization-resolved second-harmonic generation (SHG) measurements reveal a progressive suppression and eventual disappearance of the SHG signal, consistent with the restoration of inversion symmetry in the centrosymmetric AB′ phase. Complementary low-frequency Raman spectroscopy shows a pronounced stiffening of the layer-breathing (LB) vibrational mode, indicating enhanced interlayer coupling in the W-doped bilayer system compared to undoped AA-stacked samples.

Aberration-corrected scanning transmission electron microscopy (AC-STEM) provides direct insight into the spatial distribution of W dopants and correlates local compositional variations with the observed structural transformation. The results suggest that even dilute W incorporation is sufficient to energetically favor centrosymmetric stacking, thereby driving the phase transition without disrupting the overall crystalline quality. These findings establish W doping as an effective and scalable route for inducing stacking-controlled phase transitions in bilayer TMDs. Beyond fundamental insights into interlayer interactions and symmetry engineering, this approach opens new opportunities for designing phase-controlled heterostructures, tunable nonlinear optical devices, and bilayer platforms for emergent quantum phenomena, including strain- or defect-assisted single-photon emission.

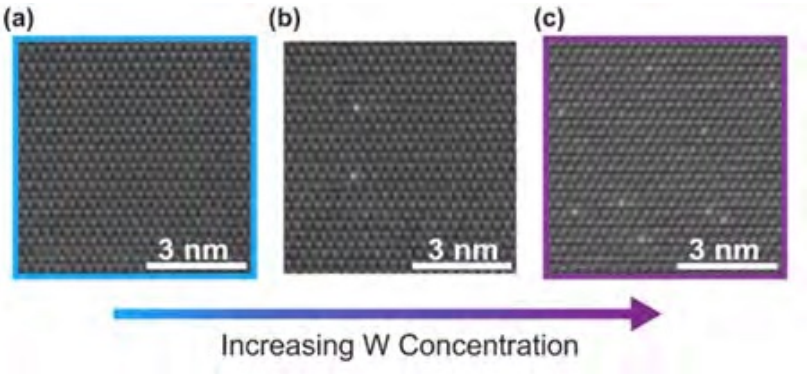


Figure 1: Different W concentrations. (a) undoped MoS_2 monolayer with no tungsten present. (b) two W atoms present within a monolayer of the MoS_2 and the increased W concentration in the bilayer shown in (c).

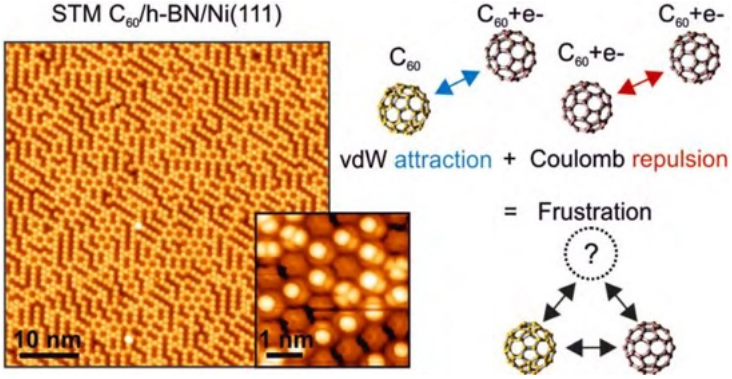
Fullerenes on Epitaxial h-BN: From ambipolar charge transfer to charge induced structural frustration

*Max Bommert, Bruno Schuler, Carlo A. Pignedoli, Gino Günzburger, Roland Widmer, Oliver Gröning**
Empa, Swiss Federal Laboratories for Materials Science and Technology, nanotech@surfaces Laboratory, 8600 Dübendorf, Switzerland.
** presenting Author: oliver.gröning@empa.ch*

Epitaxial single-layer hexagonal Boron Nitride (h-BN) grown on transition metal substrates offers a versatile platform for investigating intermolecular interactions and molecule-h-BN interfaces.[1] Its large band gap and absence of states near the Fermi energy make h-BN an ideal candidate for use as a dielectric or decoupling layer in 2D electronic devices. Recent years have witnessed a growing interest in harnessing the synergy between 2D materials and tailor-made functional molecular films to develop next-generation 2D material-organic hybrid devices.

To gain a comprehensive understanding of how molecules interact with two-dimensional materials, especially concerning energy level alignment and charge transfer mechanisms, we embarked on a project combining various fullerene sizes (C_{60}, C_{70}, and C_{84}) with two distinct h-BN transition metal systems: Rh(111) and Ni(111). The size-dependent decrease of the HOMO-LUMO gap in fullerenes in combination with the work function modulation of the substrates leads to different types of accessible charge transfer processes.[2,3]

Our investigation highlights the critical role of energy level alignment in inter-fullerene hybridization, STM-tip-induced charge transfer processes, and intrinsic charge transfer processes originating from the substrate to the fullerene. The robustness and accessibility of these charge transfer processes open pathways for the development of organic-2D material hybrid devices, capitalizing on ambipolar charge transport.



Furthermore, we discuss the complexity of adsorption configurations arising from intrinsic molecular charging, presenting a model example of charge frustration.[4] In contrast to the typical external stimuli used to influence frustrated phases (such as magnetic fields or temperature), we employ localized defect creation via STM-tip-induced manipulation to explore the electrostatic effects on the molecular ensemble.

Our study not only advances our understanding of fundamental interactions at the interface of 2D materials and organic molecules but also paves the way for innovative design strategies in emerging hybrid electronic devices.

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Phase engineering of Mn_2S_2-2D via substrate intercalation

Max Wolfertz [1], Abdallah Karaka [1], Nicolas Georgopoulos [1], Oktay Güleryüz [1], Affan Safeer [1], Thomas Michely [1], and Jeison Fischer [1]

1) II. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, 50937 Cologne, Germany

We investigate the epitaxial growth of single-layer manganese sulfide grown via molecular beam epitaxy on graphene/Ir substrates. Morphology, crystal structure and electronic properties are examined using scanning tunneling microscopy and- spectroscopy and low energy electron diffraction. While bulk MnS exists in the three polymorphs, α-(rock-salt structure), β-(zincblende structure), and γ-MnS (wurtzite structure), its structure in a single-layer is unknown, as fabrication using exfoliation methods cannot be applied. We find that when grown by molecular beam epitaxy on Gr/Ir substrates manganese sulfide grows in two competing phases: MnS in a hexagonal and a tetragonal lattice with in-plane lattice parameter 4.11 Å and 3.63 Å, respectively. We relate these phases to single layer Mn_2S_2-2D in the trigonal CuI structure (space group P-3m1) and to thin platelets of a tetragonal α-MnS (space group Fm-3m), respectively.
We show that the substrate exerts a strong influence on the phase selected, see Figure 1.
While the growth on Gr/Ir(110) results in single layer Mn_2S_2-2D , the Gr/Ir(111) substrate shows a phase coexistence dominated by the tetragonal α-MnS phase.
By intercalating Gr/Ir(111) with europium, the phase competition is removed. Stabilizing nucleation at low temperature for the new trigonal MnS phase in the single layer regime without bilayer formation.
Also, the use of seeding methods for avoiding loss of Mn into the bulk Ir crystals is discussed.

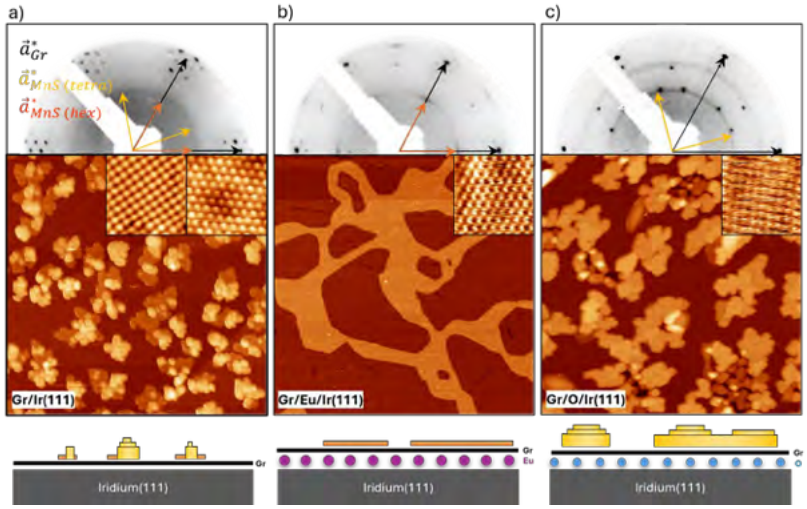

Figure 1: STM and LEED of MnS grown on different substrates. Mn was deposited in S atmosphere at 300K and annealed to a) 400K, b) 600K, c) 600K. a) Growth on Gr/Ir(111) reveals a phase coexistence of both tetragonal MnS and trigonal Mn_2S_2-2D. b) Intercalation of Gr/Ir(111) with europium prior deposition stabilizes the nucleation of trigonal Mn_2S_2-2D with apparent height of ~0.5 nm. Mn_2S_2-2D is stable for annealing temperatures up to 700K. c) oxygen-intercalation of the substrate favors the formation of bulk tetragonal MnS. LEED: 110eV, STM images: 150 x 150 nm^2 , V_{bias} = 2V, I_{set} = 50pA.

Spatially-resolved photoemission at the SGM4 beamline of ASTRID2

Alfred. J. H. Jones[1], Paulina Majchrzak[1], Zhihao Jiang[1], Chakradhar Sahoo[1], Steinn Ýmir Ágústsson[1], Davide Curcio[1], Davide Mottin[2], Panagiotis Karras[2], Søren V. Hoffman[1], Nykola C. Jones[1], Jill Miwa[1], Søren Ulstrup[1], Philip Hofmann[1]

1) Department of Physics and Astronomy, Aarhus University, 8000 Aarhus C, Denmark
2) Department of Computer Science, Aarhus University, 8000 Aarhus C, Denmark

Increased scientific interest in layered Van der Waals crystals, including their heterostructures and operational devices incorporating them, necessitates measurement techniques capable of isolating clear electronic structure signals from such small and complex systems. Here, we present our new spatially-resolved ARPES beamline at the ASTRID2 synchrotron, where a <3 μm beam spot is produced using an achromatic, elliptical capillary optic. We describe the layout of this beamline and the innovations necessary to precisely utilize the small beam for ARPES measurements. We demonstrate the capability of this beamline using nanoARPES measurements on several example systems and discuss in detail the performance of the capillary optic.

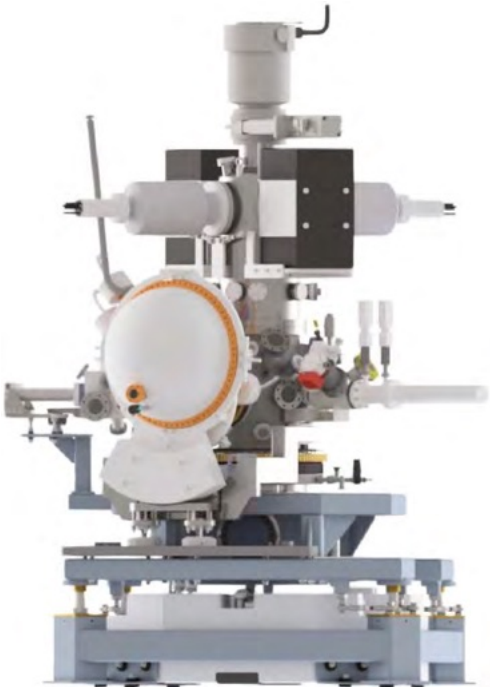

Figure 1: A model of the SGM4 spatially resolved ARPES endstation

MicroARPES study of contact doping of WSe_2 by $RuCl_3$

Thomas Nielsen[1], Edvard Solbrekken[1], Alfred J. H. Jones[1], Zhihao Zhiang[1], Chakradar Sahoo[1], Kenji Watanabe[2], Takashi Taniguchi[2], Jill A. Miwa[1], Søren Ulstrup[1]
1) Aarhus University, Denmark
2) National Institute for Materials Science, Japan

Placing van der Waals materials into contact with α-$RuCl_3$ has recently emerged as a method of modulating their electronic structures. The proximity to α-$RuCl_3$ has been observed to produce strong hole doping in the van der Waals material. [1] And this has been established as a method to create better electrical contacts in transistor devices based on monolayer transition metal dichalcogenides (TMDs). [2,3] Here, we use the ASTRID2 synchrotron light source at Aarhus University in Denmark to measure angle resolved photoemission spectroscopy (ARPES) with micron spatial resolution to study the valence bands and core levels of semiconducting monolayer TMDs in proximity to α-$RuCl_3$. We observe large valence band shifts of 0.7-0.8eV indicating a strong hole doping, placing the valence band maximum at the fermi level. The samples are produced through mechanical exfoliation with a dry-transfer stacking procedure. α-$RuCl_3$ is highly sensitive to the temperatures and chemicals typically used in the fabrication procedures of van der Waals heterostructures. How the degradation of α-$RuCl_3$ affects the proximity induced doping of the TMD is discussed based on the ARPES and XPS measurements.

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Tuning Metallic Edge States and Band Bending in Quasi-Freestanding MoS_2 via Edge Termination

Alice Bremerich,[1] Marco Thaler,[2] Mahdi Ghorbani-Asl,[3] Thais Chagas,[1] Christoph Schuster,[1] Dina Wilks,[1] Laerte Patera,[2] Arkady V. Krasheninnikov,[3] and Carsten Busse[1]

1) Universität Siegen, Germany
2) Universität Innsbruck, Austria
3) Helmholtz-Zentrum Dresden-Rossendorf, Germany

MoS_2 is the prototypical semiconducting single-layer transition-metal dichalcogenide (TMDC). It exhibits a metallic state localized at island boundaries that induces partial charge accumulation, resulting in band bending. This 1D state acts as a barrier for electron transport across the edges and plays a crucial role in quantum confinement in TMDC nanostructures. In this study, we tune the edge state and the associated band bending by altering the chemical termination of MoS_2 islands on graphene /Ir(111).

Quasi-freestanding MoS_2 is grown on graphene /Ir(111) by molecular beam epitaxy (MBE). We prepare hexagonal islands that exhibit two geometrically different edge types (Mo- and S-type). By varying the chemical potential of sulfur during growth, we modify the edge chemistry. We investigate the resulting changes in the electronic structure by scanning tunneling microscopy and spectroscopy (STM and STS) at 8 K. We find that the partial charge accumulation depends sensitively on the type of edge as well as edge chemistry, leading to distinct variations in the upward bending of both valence and conduction band.

To model the observed band bending, we employ a screened electrostatic potential generated by an infinite line charge located at the edges of the islands [1]. Density functional theory (DFT) calculations support the experimental results.

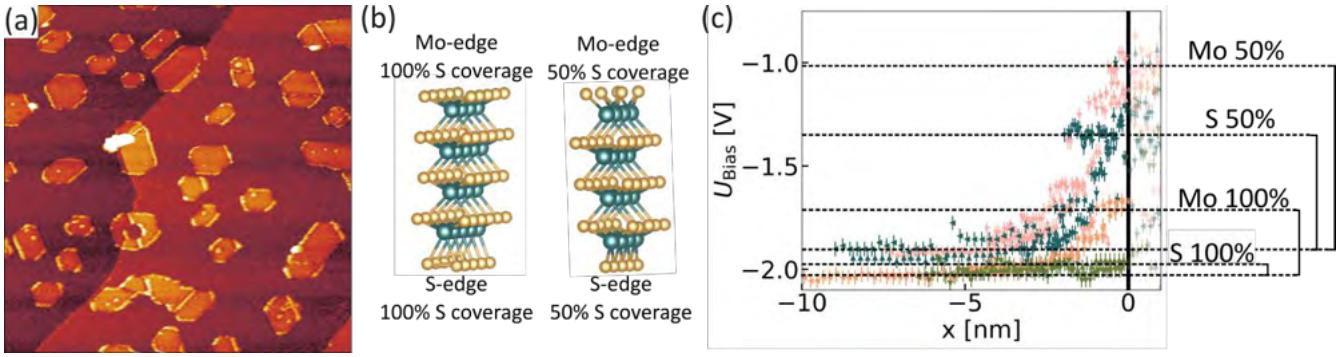

Figure 1: (a) STM image of hexagonal MoS_2 islands on graphene/Ir(111) with bright S- and dark Mo- edges. STM parameters: V_{bias} = -1.5 V, I_t = 20 pA, image size 200 × 200 nm^2. (b) Atomic schematic of reconstructed S- and Mo-edges with 100% and 50% S coverage. S and Mo atoms are depicted in yellow and blue, respectively. (c) Band bending of the valence band at the Γ-point. Pink (blue) data correspond to Mo-(S-)edge with 50% sulfur coverage and orange (green) data correspond to Mo-(S-)edge with 100% sulfur coverage. The edge position is at x = 0 nm. STS parameters: V_{st} = -2.5 V, I_{st} = 5 pA, V_{mod} = 30 mV.

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Photoemission measurements on the mixed transition metal dichalcogenides $Co_{0.25}NbSe_{(2-y)}S_y$

J. J. Flounders[1], D. Hache[1], A. Jones[1], Y. Hwang[2], . Mazzola[3] and J.A. Miwa[1]

[1] *Dept. of Physics & Astronomy, Interdisciplinary Nanoscience Center, Aarhus University, Denmark*
[2]*Electricity & Electronics & Semiconductor Applications, Ulsan College, Republic of Korea*
[2] *Dipartimento di Fisica e Astronomia "Galileo Galilei", University of Padua, IT-35131 Padua, Italy*

Altermagnets are new type of material which due to their crystalline structure show net-zero magnetization like antiferromagnets but exhibit spin-polarized band splitting due to their crystal structure such as ferromagnets [1]. Recently this phenomenon has been discovered in doped transition metal dichalcogenides (TMDs) specifically in the Co-intercalated superconducting 2H-NbSe2 polymorph [2]. This discovery coincides with the advent of a new type of TMDs, the mixed TMDs, here a second type of dichalcogenide replaces, depending on the doping, some of the original dichalcogenide whilst being intercalated with a second transition metal [3]. In this study we investigate the electronic and chemical structure through angle resolved photoemission spectroscopy with micron spatial resolution and X-ray photoemission spectroscopy of the mixed TMDs $Co_{0.25}NbSe_{(2-y)}S_y$. In $Co_{0.25}NbSe_{(2-y)}S_y$ sulphur acts as the dopant and replaces some of the selenide atoms as shown in Fig.1 a), whilst cobalt is intercalated in between the layers which is shown in Fig.1 b), together with the measuring setup. We find that the electronic structure varies between the different chalcogen stoichiometries, with one measured sample showing a similar electronic structure to $Co_{0.25}NbSe_2$ whilst another surprisingly displayed a flatband which may arise from quantum interference [4]. This flatband may be topological in nature and lies ~680meV below the fermi level and can be seen in the Γ-K direction. These observed features could suggest the possibility of hosting such fascinating effects such as the quantum Hall effect giving more insight to the emerging field of altermagnets [1].

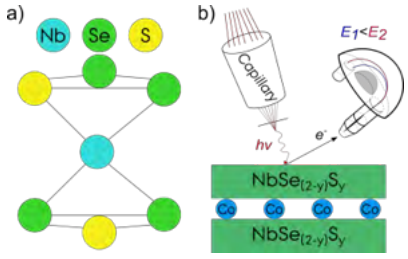

Figure 1: a) Ball and stick model representation of the mixed TMD $Co_{0.25}NbSe_{(2-y)}S_y$ 2H crystalline structure with randomised replacements of Se with S. b) Schematic of the photoemission measurements done on $Co_{0.25}NbSe_{(2-y)}S_y$, where photons with energy hv are focused by a capillary onto the sample such that a photoelectron is ejected towards the hemispherical analyser.

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Electronic and magnetic states of $CoPS_3$: Insights from experiments and theory

Yuriy Dedkov and Elena Voloshina

1) Center for Advanced Laser Techniques, Institute of Physics, 10000 Zagreb, Croatia
2) Division of Theoretical Physics, Ruđer Bošković Institute, 10000 Zagreb, Croatia

Recent breakthroughs and achievements in the studies of 2D materials have led to the increased attention to the respective van der Waals parent compounds. Herein, the class of layered materials – so-called transition metal phosphorus trichalcogenides (MPX_3; M: transition metal, X: chalcogen) – has been recently investigated extensively due to the diversity in their properties depending on the M/X combination.

Layered $CoPS_3$ can be considered as a representative example of this class of materials. Following the description according to the Goodenough-Kanamori rules, $CoPS_3$ is an antiferromagnetic material with a Néel temperature of $T_N \approx 120$ K, where direct antiferromagnetic nearest-neighbor exchange of Co^{2+} magnetic moments strongly prevails over the indirect Co−S−Co exchange. The recent systematic electron spectroscopy studies using near-edge X-ray absorption fine structure spectroscopy (NEXAFS) and resonant photoelectron spectroscopy (ResPES) combined with density functional theory (DFT) calculations allowed to assign MPX_3 materials with different M to various types of insulators, Mott-Hubbard or charge transfer [1]. Here, vdW $CoPS_3$ was assigned to the intermediate case of the mixed insulating state with $U_{dd} \approx \Delta$ [2], which was also later confirmed by the detailed band-structure mapping using angle-resolved photoelectron spectroscopy (ARPES) [3] (U_{dd} is the d–d on-site correlation energy and Δ is the charge transfer energy between the d states of the metal and the p states of the ligand/chalcogen).

By using scanning probe microscopy (AFM and STM) in combination with DFT calculations, we investigate the real-space structure of van der Waals material $CoPS_3$ down to the atomic level [4]. We observe that the voltage dependence of scanning tunneling microscopy imaging shows distinct atomic signatures, which, upon comparison to the density functional theory results, can be directly attributed to different orbital contributions. The observed orbital fingerprints suggest the high spin ground state for Co^{2+} ions (S= 3/2) and energy-dependent hybridization effects between atomic orbitals of Co, P, and S, thus providing valuable insight into the magnetic and electronic states of this van der Waals material.

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A virtual super-moiré: single layer $MnBr_2$ on graphene on Ir(110)

Affan Safeer[1], Oktay Güleryüz[1], Nicolae Atodiresei[2], Wouter Jolie[1], Thomas Michely[1], Jeison Fischer[1]

[1] *II. Physikalisches Institut, Universität zu Köln, Zülpicher Straße 77, 50937 Köln, Germany*

[2] *Peter Grünberg Institut (PGI-1), Forschungszentrum Jülich, Wilhelm-Johnen-Straße, 52428 Jülich, Germany*

Single layer $MnBr_2$ on Gr/Ir(110) constitutes a three lattice system, giving rise to a super-moiré pattern – a moiré of moirés. The super-moiré of Gr/$MnBr_2$/Ir(110) is unique, as it involves a virtual moiré of $MnBr_2$ with the Ir(110) surface lattice – two lattices not in contact with each other. Moreover, it is a first example of a super-moiré created from lattices with different symmetry: while Gr and $MnBr_2$ are of hexagonal, Ir(110) is rectangular. Using a careful Fourier analysis of the bias dependence of scanning tunneling microscope topographs, scanning tunneling spectroscopy, the known properties of Gr/Ir(110) [1], and the results of ab initio calculations, the origin of the virtual moiré is uncovered and related to the inhomogeneous binding of Gr to Ir(110) [2]. Comparative experiments with $MnBr_2$ on Gr/Ir(111) show similar growth and structure as on Gr/Ir(110), but highlight the unique properties of the $MnBr_2$/Gr/Ir(110) super-moiré.

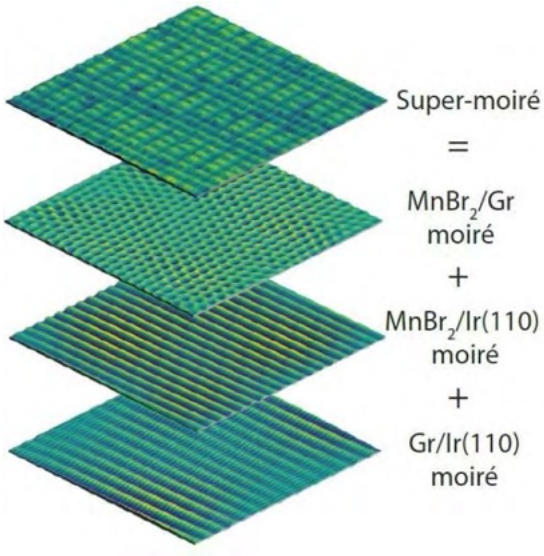

Figure 1: Schematic representation of how the supermoiré of $MnBr_2$/Gr/Ir(110) evolves by superposition of three moirés, including the virtual moiré with Ir(110) and $MnBr_2$.

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Potential Altermagnetic Splitting in $Fe_{0.25}WSe_2$

Dominic Hache[1], John Flounders[2], Alfred Jones[1] Søren Ulstrup[1], Philip Hofmann[1], Younghun Hwang[4], Federico Mazzola[3] and Jill Miwa[1]

1) Department of Physics and Astronomy, Aarhus University, Aarhus, Denmark.

2) iNano, Aarhus University, Aarhus, Denmark.

3) Department of Physics and Astronomy 'Galileo Galilei", University of Padova, Padova, Italy.

4) Electricity and Electronics and Semiconductor Applications, Ulsan College, Ulsan 44610, Republic of Korea.

Rising power demands from artificial intelligence and other emerging technologies motivate the search for more energy-efficient electronic platforms. Spintronics provides one possible route by exploiting the electron spin degree of freedom, with altermagnetic materials offering a particularly intriguing opportunity to realize spin-split electronic bands without net magnetization. In these systems, symmetry breaking associated with long-range magnetic order can lift spin degeneracies at selected points in the Brillouin zone, potentially enabling spin-selective transport phenomena. Here, we investigate the transition metal dichalcogenide $Fe_{0.25}WSe_2$, which exhibits antiferromagnetic order below approximately 55 K and may show an associated band opening near the M point. These findings suggest that $Fe_{0.25}WSe_2$ could provide a useful layered-material platform for investigating possible altermagnetic behaviour.

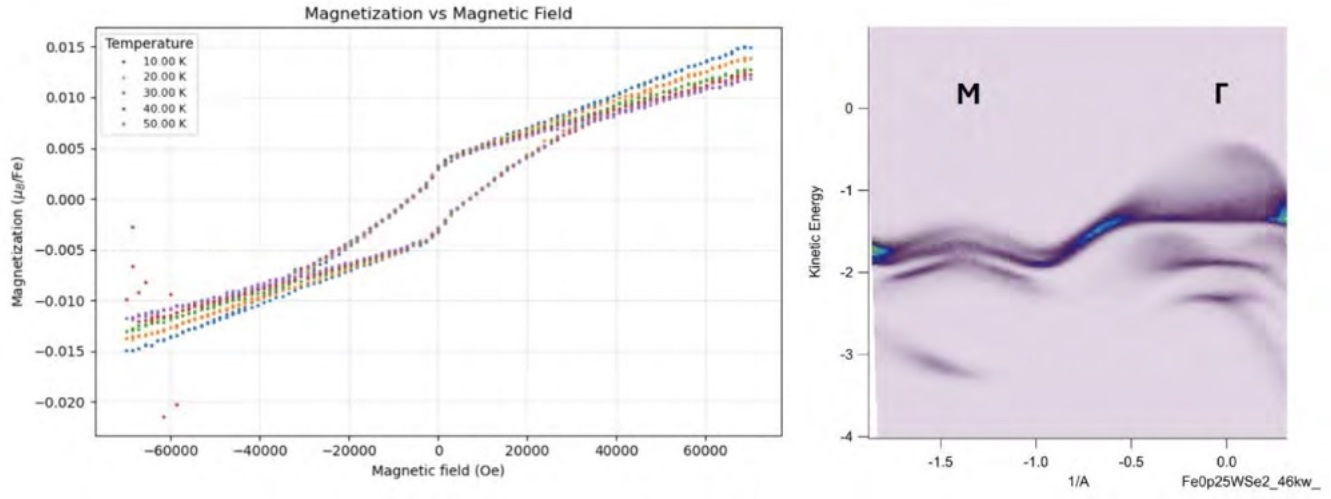

Figure 1: Magnetization in an external field suggests antiferromagnetic order with canted spins (left). ARPES data acquired at 35 K where the splitting of the bands is visible at the M point (right).

Quantifying Surface Contamination of Graphene

Carolin Frank,[1,2] Kevin Vomschee,[1] Barbara Maria Mayer,[1] Harriet Åhlgren,[1] Marika Schleberger,[2] and Daniel Primetzhofer[1,3]

1) Materials Physics, Department of Physics and Astronomy, Uppsala University, Uppsala, Sweden
2) Faculty of Physics and CENIDE, University of Duisburg-Essen, Duisburg, Germany
3) Tandem Laboratory, Uppsala University, Uppsala, Sweden

Surface contamination represents a major challenge in surface science, as it strongly affects the intrinsic properties of two-dimensional materials, including doping levels and thermal conductivity. Since the discovery of graphene in 2004, numerous ex-situ and in-situ cleaning methods have been developed, such as thermal annealing, or laser- and plasma-based treatments. While contamination can be identified at the atomic scale using techniques such as transmission electron microscopy [1], quantitative determination of contamination remains challenging.

To address this issue, we developed a method to quantify contamination of graphene based on recoil-projectile coincidence in ion scattering experiments. Specifically, we performed recoil-projectile coincidence measurements of 40 keV xenon ions transmitted through self-supporting single-layer graphene on a TEM grid using the Time-of-Flight Medium Energy Ion Scattering (ToF-MEIS) setup at Uppsala University [2].

In order to investigate the influence of sample preparation on graphene cleanliness, we compared three differently prepared graphene samples, transferred using either a PMMA-based or a PMMA-free process [3]. Our results show that graphene contamination consists predominantly of carbon and hydrogen. Among the investigated samples, the PMMA-free transferred graphene exhibits the lowest native levels of both carbon and hydrogen contamination.

Furthermore, we studied the effect of in-situ thermal annealing in UHV conditions on the cleanliness of graphene by annealing the samples to a nominal temperature of 400°C for 1h. Immediately after annealing, contamination was found to be completely removed for all samples. While carbon and hydrogen contamination rapidly reappear on PMMA-transferred samples, the PMMA-free transferred sample remains nearly contamination-free even 100 minutes after annealing.

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"Room-Temperature Synthesis of 2D $Ti_3C_2T_x$ MXene Nano-sheets via Organic Base Treatment for Rechargeable Alkali-Metal Battery Electrodes"

Sunaina Rafiq,[1] Alessandra Gentili,[2] Maria Assunta Navarra,[2] Maria Grazia Betti,[1] and Carlo Mariani [1]

1) Dipartimento di Fisica, Sapienza Università di Roma, P.le Aldo Moro 2, 00185 Rome, Italy
2) Dipartimento di Chimica, Hydro-Eco Research Center, Sapienza Università di Roma, P.le Aldo Moro 2, 00185 Rome, Italy

Abstract:

In this work, we present a cost-effective synthesis of the novel two-dimensional (2D) multilayered $Ti_3C_2T_x$ MXene nanosheets by intercalating tetramethylammonium (TMA^+) ions at room-temperature via manual shaking, instead of using ultra-sonication methods. The TMAOH organic solvent weakens the interlayer bonds and the intercalated TMA^+ ions expands interlayer spacing by interacting with surface functional groups (-O, -OH, -F). The XRD data confirms successful synthesis of MXene ($Ti_3C_2T_x$) nano-sheets via its characteristic planes (002) and/or c-lattice expansion from 18.8 to 29.4Å. A morphological study obtained by SEM revealed the perfect layered structure of $Ti_3C_2T_x$, while EDX results shows Al removal and reduced F-content after TMAOH treatment. X-ray photoemission (XPS) data aligning with EDX study enlightens a slightly different surface composition with respect to the bulk. High-resolution Ti2p core-level spectra recorded for the compounds allow us to understand the nature of chemical bonding in all samples. Electrochemical testing with Lithium (Li^+), Sodium (Na^+), and Potassium (K^+) under identical conditions shows ion-size-dependent behavior. Voltage profile analysis revealed distinct behaviors, with Li^+ and K^+, highlighting different energy storage mechanisms. This work offers novel contributions to understanding MXene' potential for energy storage applications.

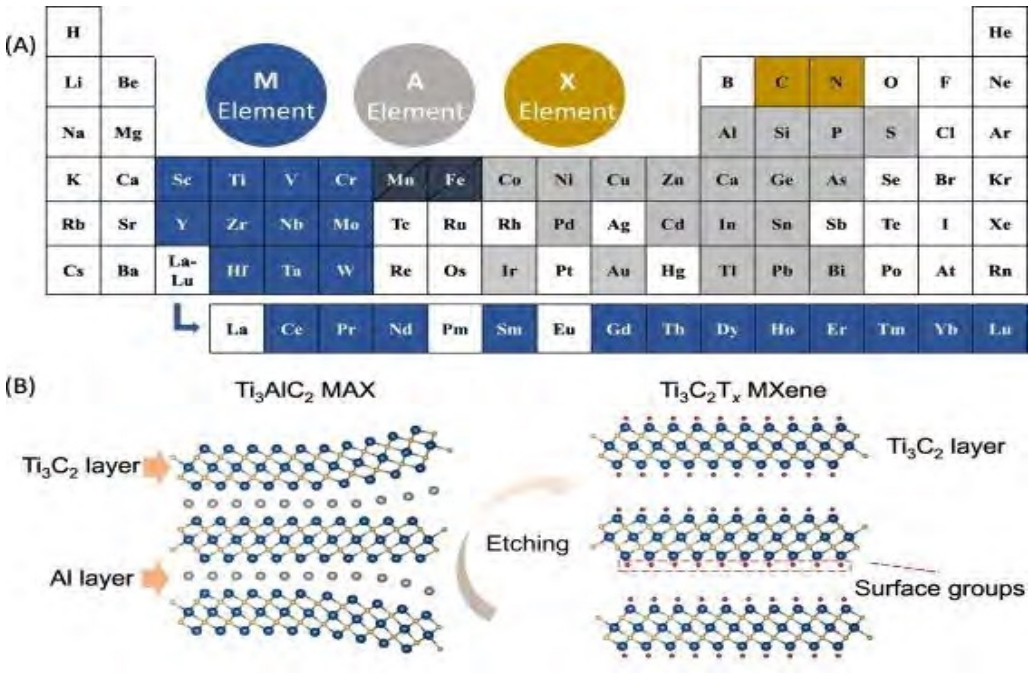

Figure 1: General idea of forming the MXene ($Ti_3C_2T_x$) nano-sheets from its MAX (Ti_3AlC_2) phase.

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Imaging Spin Filter for NanoESCA based on Au/Ir or oxide passivated Fe

Matthias Escher[1], Nils Weber[1], Timna Kühn[1], Marten Patt[1]

1) SPECS Surface Nano Analysis GmbH, 13355 Berlin, Germany

Energy-filtered photoelectron microscopes have been used for various applications including work-function mapping, imaging XPS and in the last years more prominently for imaging the reciprocal space, i.e., momentum microscopy. A big advantage of momentum microscopy is that it projects the sample surface in real space as well as the angular distribution (ARPES) of the electrons. This allows us to study electronic properties, including spin properties of graphene and 2D materials on locally defined sample regions [1]. Spin-resolved Momentum Microscopy can be used to engineer the spin-polarized electronic structure of two-dimensional half-metals [2] and other 2D materials [3].

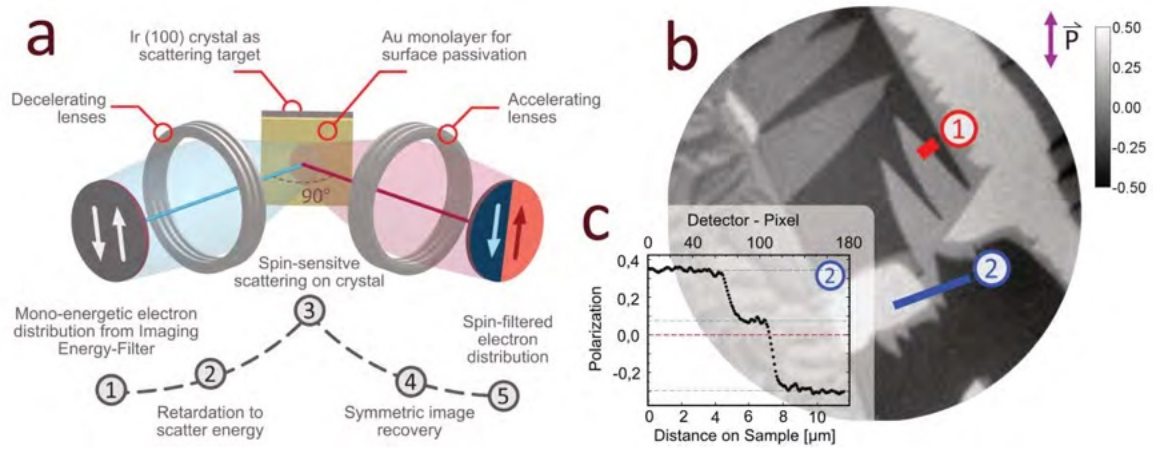

Figure 1: The monochromatic electron image delivered by the NanoESCA is spin-filtered by a scattering process (a) which allows to measure the spin polarization of the whole image simultaneously, e.g. magnetic domains of a poly-crystalline iron film (b). The field-of-view of this real-space microscopy image was set to a diameter of 66 µm. Line-scans along the domain boundaries (c) show the contrast and precision of the method.

The Focus NanoESCA [4] MARIS analyzers and imaging spin-filters in combination with powerful UV light sources and system bases of SPECS are comprehensive tools for spin-related research. With imaging spin-filters, the effective 2D figure-of-merit, thus its detection efficiency, is increased by nearly four orders of magnitude compared to single-channel spin detectors [5]. We also present proof of principal measurements of an Imaging Spin Filter with oxide passivated Fe as scattering target, which is a way to switch the polarization detection direction of these filters easily.

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