Wrocław University
of Science and Technology

Flatlands

September 9-13, 2024
Wroclaw, Poland

Book of abstracts

Program

Sunday

18:00 - 20:00 Welcome reception

Monday

8:45 Opening

2D materials for interaction with molecules

Chair: Matt Beard

9:00 (I1) **Reshef Tenne** Catalytic processes aided by 2D-materials

9:30 (C1) **Johannes Binder** Wafer-scale Hexagonal Boron Nitride for Hydrogen Generation by Radiolysis of Interfacial Water

9:45 (C2) **Mohsen Beladi Mousavi** Ion Transport Dynamics in Single MXene Nanoparticles Revealed by Interferometric Scattering Microscopy

10:00 Coffee break

Magnetic 2D materials

Chair: Alexander Högele

10:30 (I2) **Amine Ben Mhenni** Bose-Fermi mixture in a strongly correlated moiré bilayer electron system

11:00 **Sami Mitra** (Editor of Physical Review Letters)

11:15 (C3) **Aleksandra Łopion** Collosal field-induced energy shift of higher-energy excitons in CrSBr

11:30 (I3) **Maciej Molas** Excitons and phonons in van der Waals materials

12:00 Lunch break

Theory of 2D materials

Chair: Christoph Gadermaier

13:30 (I4) **David A. Egger** Anharmonicity and Optoelectronic Properties of Halide Perovskites: from 3D to 2D

14:00 (C4) **Yilyu Guo** Laser-induced ultrafast spin injection in all-semiconductor magnetic CrI_3/WSe_2 heterobilayer

14:15 (C5) **Agnieszka Kuc** Strong Dipolar Repulsion of One-Dimensional Interfacial Excitons in Monolayer Lateral Heterojunctions

14:30 (I5) **Ermin Malic** Optics and dynamics of excitons and trions in 2D materials

15:00 Coffee break

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Program

Monday

2D materials straintonics

Chair: Kirill Bolotin

15:30 (I6) **Elena Blundo** Strain in Flatlands

16:00 (C6) **Thomas Brumme** Understanding the Impact of Non-Uniform Strain Fields on Exciton Dynamics in Multilayered 2D Transition Metal Dichalcogenides

16:15 (C7) **Michele Gastaldo** Tunable strain and bandgap in subcritical-sized MoS2 nanobubbles

16:30 (I7) **Carmen Munuera** Insights into MoS2-based devices via operando Scanning Probe Microscopy

Tuesday

2D materials mechanics

Chair: Christoph Stampfer

9:00 (I8) **Kirill Bolotin** Nanomechanical probing, manipulation, and control of excitons in 2D materials

9:30 (C8) **Dipanjan Sen** Integration of Ferroelectric and Freestanding 3D $SrTiO_3$ and 2D MoS_2 Nanomembranes for Multifunctional Devices

9:45 (C9) **Emeline Nysten** Acousto-Optoelectric Spectroscopy on Transition Metal Dichalcogenides with Surface Acoustic Waves

10:00 Coffee break

Complex 2D materials systems

Chair: Christian Schneider

10:30 (I9) **Alexander Högele** Exciton, charge and spin lattices in moiré heterostructures

11:00 (C10) **Bo Han** UInfrared Magneto-Polaritonics And In-Situ Tuning of Exciton Dynamics In Two-Dimensional Crystals And Heterostructures In a Cryogenic Open Cavity

11:15 (C11) **Subir Ghosh** Monolithic and heterogeneous three-dimensional (3D) integration of two-dimensional (2D) materials using dense vias

11:30 (I10) **Christoph Stampfer** Electrostatically defined quantum dots in bilayer graphene

12:00 Lunch break

⋮

Program

Tuesday

Complex light-2D materials interactions

Chair: Ursula Wurstbauer

13:30 (I11) **Tomasz Smoleński** Correlated kinetic magnetism of electrons in semiconductor moiré materials

14:00 (C12) **Doron Naveh** Exploring Light - Matter Interactions at the Interface of a 2D Antiferromagnetic Semiconductor Heterojunctions

14:15 (C13) **Álvaro Moreno Abajo** Harnessing TBG for enantiomeric sensing of chiral molecules

14:30 (I12) **Matthew Beard** Controlling Spins using Chiral 2D Perovskite Semiconductors

15:00 Coffee break

Excitons in 2D materials I

Chair: Maciej Molas

15:30 (I13) **Christian Schneider** Controlling Excitons in van-der-Waals materials in tunable optical cavities

16:00 (C14) **Jamie Fitzgerald** Circumventing the polariton bottleneck via dark excitons in 2D semiconductors

16:15 (C15) **Jakub Jasiński** Quadrupolar Excitons in Natural $MoSe_2$ Bilayer

16:30 (I14) **Ursula Wurstbauer** Moiré Minibands, twist disorder and exciton-phonon coupling in van der Waals stacks

17:00 (- 18:00) Shotgun - Chair: Alexey Chernikov

18:15 (- 20:00)
Poster session I (P1 - P25)

Wednesday

Hybrid and magnetic 2D materials

Chair: Efrat Lifshitz

9:00 (I15) **Will Tisdale** Hybrid Organic-Inorganic 2D materials

9:30 (C16) **Muhammad Zubair Khan** Layer dependent magnetic ordering in two-dimensional magnetic insulator

9:45 (C17) **Łucja Kipczak** Magnetic proximity interactions in the $CrCl_3$/hBN/WSe_2 heterostructures

10:00 Coffee break

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Program

Wednesday

Anisotropic and hybrid 2D materials

Chair: William Tisdale

10:30 (I16) **Alexey Chernikov** Manipulation and transport of excitons in 2D semiconductors and antiferromagnets

11:00 (C18) **Nirman Chakraborty** Inversion of magnetic anisotropy in thermally intercalated few-layer transition-metal thiophosphates: a magneto-optical investigation

11:15 (C19) **Vojtech Kundrat** Exotic core-shell nanotubes synthesized via Van der Waals epitaxy

11:30 (I17) **Alexander Urban** Low-dimensional halide perovskite emitters – Accelerated discovery and enhanced optical properties

12:00 Lunch break

Atomic defects and synthesis

Chair: Carmen Munuera

13:30 (I18) **Hong-Hua Fang** Quantum Emitters in van der Waals layered materials

14:00 (C20) **Harikrishnan Ravichandran** Exploiting Point Defects in Two-dimensional Materials for Stochastic Encoding

14:15 (C21) **Lorena Manzanares** Distance Dependence of Mxene-Induced Fluorescence Energy Transfer and Applications in Single Molecule Biosensing

14:30 (I19) **Zdenek Sofer** Xenes - chemistry beyond graphene

15:00 (I20) **Adina Luican-Mayer** Quantum Functionality in 2D materials: From Moiré Structures to Quantum Confined Devices

17:00 Boat trip

18:00
Conference banquet

Thursday

Magnetic 2D materials

Chair: Tomasz Smoleński

9:00 (I21) **Efrat Lifshitz** Magneto-optical properties in the vdWs $NiPS_3/WSe_2$ heterostructure

9:30 (C22) **Farsane Tabataba-Vakili** Doping-control of excitons and magnetism in few-layer CrSBr

9:45 (C23) **Maciej Śmiertka** High Energy Magnetic Excitons In CrSBr

10:00 Coffee break

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Program

Thursday

Theory of 2D materials

Chair: Adina Luican-Mayer

10:30 (I22) **Kristian Thygesen** Data-driven discovery of novel 2D materials

11:00 (C24) **Rico Friedrich** Magnetic Properties of Non-van der Waals 2D Materials

11:15 (C25) **Anas Siddiqui** Understanding Domain Reconstruction of Twisted Bilayer and Heterobilayer Transition Metal Dichalcogenides through Machine Learned Interatomic Potentials

11:30 (I23) **Thomas Heine** Everything you always wanted to know about bilayers

12:00 Lunch break

Optoelectronics of 2D materials

Chair: Saptarshi Das

13:30 (I24) **Joanna Jadczak** Photon upconversion in monolayer transition metal dichalcogenides

14:00 (C26) **Ashish Arora** Giant Faraday Rotation in 2D Semiconductors

14:15 **EUROTEK**

14:30 (I25) **Goki Eda** Spontaneous photovoltaic effect in polar 2D materials

15:00 Coffee break

2D material devices

Chair: Goki Eda

15:30 (I26) **Saptarshi Das** 3D Integration of 2D Devices for Advanced Memory, Logic, and Bio-inspired Computing

16:00 (C27) **Aljosha Söll** High-κ Wide-Gap Layered Dielectric for Two-Dimensional van der Waals Heterostructures

16:15 (C28) **Hongde Yu** Metal-free magnetism in two-dimensional polymers

16:30 (C29) **Mayukh Das** Substitutional dopant engineering to achieve High-performance p-type Two-dimensional Field Effect Transistors

16:45 (C30) **Yigit Sozen** Fabrication of high performance WSe_2 phototransistors and Si/MoS_2 pixel image sensors with High-Throughput Mechanical Exfoliation

17:00 (- 18:00) Shotgun - Chair: Thomas Heine

18:15 (- 20:00)
Poster session II (P26 - P51)

Program

Friday

Excitons in 2D materials II

Chair: Joanna Jadczak

9:00 (I27) **Andras Kis** Exciton Manipulation and Transport in 2D Semiconductor Heterostructures

9:30 (C31) **Natalia Zawadzka** Linearly-polarized electroluminescence in van der Waals heterostructures

9:45 (C32) **Thomas Pucher** Freestanding Ferroelectric Perovskite Oxides: from High performance Transistors to Tunable Exciton Emission

10:00 Coffee break

Engineering and dynamics of 2D materials

Chair: Andras Kis

10:30 (I28) **Andres Castellanos** Strain engineering phase transition in $NbSe_2$

11:00 (C33) **Maya Bar Sadan** Nanotubes and Other Nanostructures of VS_2, WS_2, and MoS_2: Structural Effects on the Hydrogen Evolution Reaction

11:15 (C34) **Levna Chacko** Engineering Functionalized Mxene-based Interfaces for Superior Photocatalytic Hydrogen Evolution

11:30 (I29) **Christoph Gadermaier** Modulation of Ultrafast Quasiparticle Dynamics in Two-dimensional Semiconductors

12:00 Closing

12:15 Lunch break

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Invited presentations

I1

Catalytic processes aided by 2D-materials

Reshef Tenne

Department of Molecular Chemistry and Materials Science, Weizmann Institute,
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About 80-90% of the chemical processes running in the industry are executed with catalysts. For example, the *Haber-Bosch* process for the production of ammonia from free nitrogen is run at pressures larger than 150 bars and temperatures reaching 450 °C with iron as the main catalyst. This indispensable process is responsible for 20% of the nitrogen in our body and consumes 1% of the global energy outlay (and contributes 1-2% to the global carbon footprint). Nickel and cobalt doped MoS_2 serve as the main hydrodesulphorization and hydrodenitirization catalysts of fuel. Splitting water to oxygen and hydrogen via electrocatalysis process is among the most sought-for reactions for the projected zero-carbon footprint 2050 world. Like almost any other catalyst, 2D-materials nanoparticles (NPs) cannot be used as such for performing a useful catalytic process. One can distinguish between two types of catalysts: doped 2D-materials NPs and hybrid ones.

Several examples will be discussed in this connection in this presentation. Owing to their limited stability in oxidative environment, transition metal dichalcogenides (TMDCs) are not suitable for the electrocatalytic oxygen evolution reaction (OER). Nonetheless, they have shown promising catalytic reactivity for the hydrogen evolution reaction (HER). For example, Pt-doped MoS_2 exhibited high catalytic reactivity for the HER.[1] Similarly, Co-P doped g-C_3N_4 displayed strong photocatalytic reactivity with respect to the water splitting reaction.[2] Another example is the HER performed by core-shell hybrid MoS_2 coated gold nanoparticles (Au-NP&MoS_2)[3] and $CsPbBr_3$@MoS_2 core-shell nanoparticles.[4] The HER reactivity of the Au-NP&MoS_2 core-shell nanoparticles can be ascribed to the vectorial charge transfer from the metallic gold nanoparticles to the catalytically reactive conformal MoS_2 coating. The photocatalytic reactivity of the $CsPbBr_3$@MoS_2 core-shell nanoparticles can be attributed to the complementary absorption of the perovskite NP which is coated conformably with the MoS_2 film. Few other examples for the catalytic reactivity of 2D-materials nanoparticles will be presented and discussed in this talk.

References
1. J. Deng, et al., *Energy Environ. Sci*. **8**, 1594 (2015).
2. W. Liu, et al., *Angew. Chem., Int. Ed.* **56**, 9312 (2017).
3. R. Bar-Ziv et al., *ACS Appl. Energy Mater*. **2**, 6043 (2019).
4. A. Goldreich et al., https://doi.org/10.26434/chemrxiv-2024-zpfbx

I2

Bose-Fermi mixture in a strongly correlated moiré bilayer electron system

Amine Ben Mhenni, Wilhelm Kadow, Mikolaj Metelski, Adrian O. Paulus, Alain Dijkstra, Matteo Barbone, Jonathan J. Finley, Michael Knap, and Nathan P. Wilson

Walter Schottky Institute, TUM School of Natural Sciences, and
MCQST, Technical University of Munich, Munich, Germany

Bilayer electron systems in 2D semiconductors can host dipolar excitons, allowing the study and manipulation of bosonic phases[1,2,3]. Though they are predicted to exhibit a rich phase diagram[4], less attention has been accorded to the study of Bose-Fermi mixtures in such systems. Here, we use a WS_2/WSe_2 moiré layer, which is Coulomb-coupled to a WSe2 layer, to realize a dipolar excitonic phase that persists under electron doping. We use various excitonic probes to study the electrostatic phase diagram of this bilayer electron system and reveal a highly tunable boson/fermion fraction and asymmetric stability with respect to particle/hole doping. We use a microscopic model to explain the latter behavior, yielding a good agreement with the experiment. Our study establishes bilayer electron systems with underlying moiré patterns as an intriguing platform to study Bose-Fermi mixtures with tunable density and the potential for long-range interactions.

1. J. P. Eisenstein, A.H. MacDonald Bose–Einstein condensation of excitons in bilayer electron systems. *Nature* 432 (2004)
2. Y. Xu *et al.* Correlated insulating states at fractional fillings of moiré superlattices. *Nature* **587** (2020)
3. Gu,J. *et al.* Dipolar excitonic insulator in a moiré lattice. *Nat. Phys.* **18** (2022)
4. J. von Milczewski *et al.* Functional-renormalization-group approach to strongly coupled Bose-Fermi mixtures in two dimensions. *Phys. Rev. A* **105** (2022)

I3

Excitons and phonons in van der Waals materials

M. R. Molas

Institute of Experimental Physics, Faculty of Physics, University of Warsaw, Warsaw, Poland

Semiconducting transition metal dichalcogenides (S-TMDs) based on molybdenum and tungsten, *i.e.* MoS$_2$, MoSe$_2$, MoTe$_2$, WS$_2$, and WSe$_2$, are the most well-known representatives of van der Waals materials. Their most distinguished hallmark is the transition from indirect- to direct-band gap, when thinned down from a bulk to a monolayer (ML). The optical response of S-TMDs is caused mainly by excitonic effects, even at room temperature, due to the large excitonic binding energy at the level of hundreds of meV. Moreover, the exciton-phonon coupling (EPC) is significant in thin layers of S-TMDs, which leads to the rich Raman scattering (RS) spectra under their resonant excitation conditions.

In my talk I will give an overview on excitons and phonons apparent in high quality S-TMD MLs and bilayers (BLs) encapsulated in hexagonal BN. The first part of the lecture will cover experimental and theoretical investigations of excitonic properties in ML and the BL of MoSe$_2$ [1]. The measured magnetic field evolutions of the reflectance contrast spectra of the MoSe$_2$ ML and BL permit one to determine g-factors of intralayer A and B excitons, as well as the g-factor of the interlayer exciton. The dependence of g-factors on the number of layers and excitation state will be explained using first-principles calculations. It will be demonstrated that the experimentally measured ladder of excitonic *s* states in the ML can be reproduced using the $k\cdot p$ approach with the Rytova–Keldysh potential that describes the electron–hole interaction. On the contrary, the analogous calculation for the BL case requires taking into account the out-of-plane dielectric response of the MoSe$_2$ BL.

The second part of my talk will be devoted to the study of phonons in the four S-TMD MLs, i.e. MoS$_2$, MoSe$_2$, WS$_2$, and WSe$_2$, using Raman scattering excitation (RSE), which is an experimental technique in which the spectrum is made up by sweeping the excitation energy when the detection energy is fixed [2]. It will be shown that the outgoing resonant conditions of Raman scattering reveal an extraordinary intensity enhancement of the phonon modes, which results in extremely rich RSE spectra. The obtained spectra are composed not only of Raman-active peaks, *i.e.* in-plane E’ and out-of-plane A’$_1$, but the appearance of 1st, 2nd, and higher-order phonon modes is recognized. Moreover, the intensity profiles of the A’$_1$ modes in the investigated MLs resemble the emissions due to neutral excitons measured in the corresponding PL spectra for the outgoing type of resonant Raman scattering conditions. This results indicates that the strength of EPC in S-TMD MLs strongly depends on the type of their ground excitonic state, *i.e.* bright or dark, resulting in different shapes of the RSE spectra.

[1] Ł. Kipczak, et al., *2D Materials* **10**, 025014 (2023).
[2] M. Zinkiewicz, et al., *npj 2D Materials and Applications* **8**, 2 (2024).

I4

Anharmonicity and Optoelectronic Properties of Halide Perovskites: from 3D to 2D

David A. Egger

Department of Physics, TUM School of Natural Sciences,
Technical University of Munich, Garching, Germany

Halide perovskites (HaPs) are interesting materials for various optoelectronic applications and because they were found to show an array of peculiar physical effects. What stands out compared to many other semiconductors are strongly anharmonic lattice vibrations occurring in 3D and 2D HaPs already around room temperature. Theoretical predictions of their optoelectronic and other properties at finite temperatures are challenging as a consequence of it. This is because conventional treatments based on perturbative methods cannot account for the full scale of electron-lattice interactions in HaPs and related materials. Following our previous work on 3D HaP materials, [1-4] here I will present the impact of anharmonic lattice vibrations on optoelectronic properties of lower dimensional HaP materials including surfaces and 2D systems. Our approach starts from using molecular dynamics for calculating the finite-temperature atomic motions, including anharmonicity in the lattice dynamics. Machine learning methods are employed to accelerate these calculations, allowing us to compute the large supercells needed for the lower-dimensional cases with high accuracy. We predict dynamic changes in the optoelectronic properties through an efficient electronic-structure approach. Similarities and differences in the vibrational and optoelectronic properties of 3D and 2D HaPs will be discussed.

[1] Mayers et al., Nano Lett. 18, 8041 (2018)
[2] Schilcher et al., Phys. Rev. Mater. 7, L081601 (2023)
[3] Seidl et al., Phys. Rev. Mater. 7, L092401 (2023)
[4] Caicedo-Dávila et al., Nature Commun. 15, in print (2024)

I5

Optics and dynamics of excitons and trions in 2D materials

Ermin Malic

University of Marburg, Physics Department, Ultrafast Quantum Dynamics Group, Germany

Monolayer transition metal dichalcogenides (TMDs) and related van der Waals heterostructures exhibit a rich exciton and trion landscape including bright and a variety of dark states as well as spatially separated interlayer and layer-hybridized exciton and trion states. Solving 2D material Bloch equations for excitons, trions, phonons and photons, we obtain a microscopic access to the interplay of optics, dynamics and transport phenomena in these technologically promising materials.

In joint theory-experiment studies, we shed light on:

- importance of dark hybrid excitons on the charge transfer dynamics and the formation of interlayer excitons in TMD heterostructures [1-2],
- appearance of a relaxation bottleneck drastically slowing down the relaxation cascade of moiré excitons at low twist angles [3], and
- photoluminescence signatures of electrically tunable layer-hybridized trions in doped TMD homobilayers [4-5].

The gained microscopic insights are crucial for understanding and controlling many-particle phenomena governing exciton optics, dynamics and transport in technologically promising 2D materials and related heterostructures.

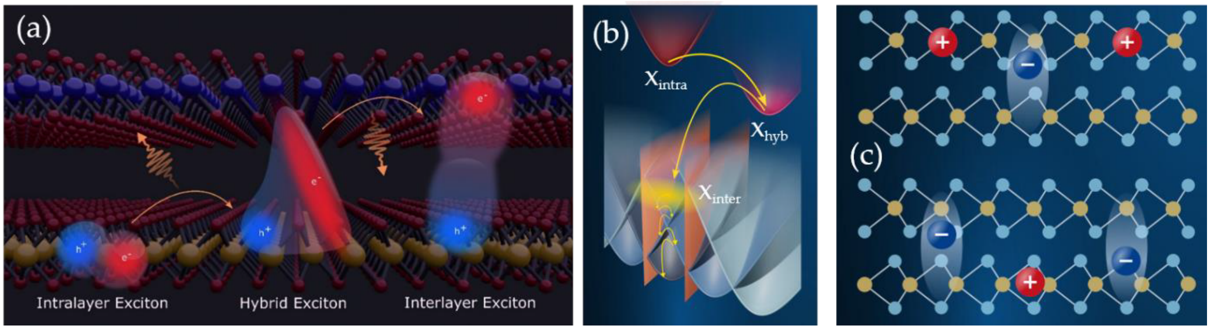

Fig. 1: (a) Sketch of the phonon-driven charge transfer process via dark hybrid excitons in a TMD heterostructure. (b) Formation of hot interlayer excitons and their relaxation cascade. (c) Layer-hybridized trions in a p- and n-doped TMD homobilayer.

[1] D. Schmitt, G. Meneghini, E. Malic, S. Hofmann, M. Reutzel, S. Mathias, et al., Formation of moiré interlayer excitons in space and time, Nature **608**, 499 (2022)

[2] J. Bange, G. Meneghini, E. Malic, M. Reutzel, S. Mathias, et al., Probing electron-hole Coulomb correlations in the exciton landscape of a twisted semiconductor heterostructure, Sci. Adv. **10**, eadi1323 (2024)

[3] G. Meneghini, S. Brem, E. Malic, Excitonic thermalization bottleneck in twisted TMD heterostructures, Nano Lett. **24**, 4505 (2024)

[4] R. Perea-Causin, S. Brem, O. Schmidt, E. Malic, Trion photoluminescence and trion stability in atomically thin semiconductors, Phys. Rev. Lett. **132**, 036903 (2024)

[5] Electrically tunable layer-hybridized trions in doped WSe_2 bilayers, R. Causin, S. Brem, F. Buchner, K. Watanabe, T. Taniguchi J. Lupton, K. Lin, E. Malic, ArXiv: 2404.18716 (2024)

I6

Strain in Flatlands

E. Blundo [1], F. Tuzi [1], S. Cianci[1], G. Pettinari[2], M. Felici[1] and A. Polimeni[1]

[1] *Physics Department, Sapienza University of Rome, Piazzale A. Moro 5, 00185 Rome, Italy.*
[2] *Institute for Photonics and Nanotechnologies, CNR, via Fosso del Cavaliere 100, 00133 Rome, Italy.*

van der Waals (vdW) two-dimensional (2D) materials exhibit intriguing and peculiar properties, that can be tuned to make them suitable for fundamental research and for applications. Despite their atomic thickness, 2D materials feature an outstanding mechanical robustness and resilience, so that mechanical deformations represent one of the most viable and effective tools to engineer their properties. Here, we show how strain can be exploited in 2D materials and heterostructures (HSs) to fine-tune their optoelectronic properties and to engender novel effects.

Strain is here induced in several 2D materials, with the focus being on semiconducting transition-metal dichalcogenides (TMDs), by an original approach consisting in the creation of nano- and micro-domes filled with highly pressurised hydrogen [1] (Fig. 1a). TMD domes are thick just 1 layer and host complex strain fields that increase while going from their edge towards their centre, reaching remarkably high values of about 5%. Such high strains cause dramatic changes in the electronic properties of the materials, such as a strain-induced direct-to-indirect bandgap transition [2] (Figs. 1b-c) and hybridisation phenomena between direct and indirect excitons [3]. The effects of strain are further investigated towards the achievement of ordered arrays of quantum emitters [4] (Fig. 1d), and towards the realisation of vdW HSs with yet novel properties. Specifically, we show how strain can be exploited to activate the electronic coupling of TMDs with InSe, leading to the achievement of a type-I alignment with an unprecedentedly efficient carrier tunnelling between the TMD and InSe, resulting in a giant photoluminescence enhancement of InSe (Fig. 1e).

Our results demonstrate the great potential of strain to create exciting new avenues in Flatlands.

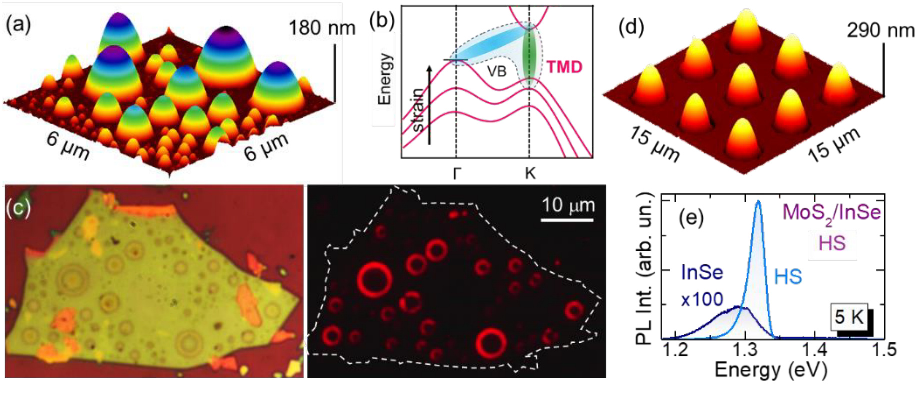

Fig. 1. (a) Atomic force microscope (AFM) image of TMD domes. (b) Sketch of the band structure of TMD MLs highlighting a strain-induced direct (green) to indirect (cyan) exciton transition. (c) Optical image of a WS$_2$ flake with domes (left) and of the photoluminescence (PL) emitted by the same sample (right). The PL is dominated by the direct (indirect) exciton towards the dome edge (centre), resulting in a ring-like PL pattern. (d) AFM image of an ordered array of MoS$_2$ domes. (e) PL signal of a InSe/strained-MoS$_2$ HS and comparison with the PL of the bare InSe flake, revealing a giant PL enhancement in the HS.

[1] D. Tedeschi, E. Blundo et al., *Advanced Materials* **31**, 1903795 (2019).
[2] E. Blundo et al., *Physical Review Research* **2**, 012024 (2020).
[3] E. Blundo et al., *Physical Review Letters* **129**, 067402 (2022).
[4] S. Cianci et al., *Advanced Optical Materials* **11**, 2202953 (2023).

I7

Insights into MoS_2-based devices via operando Scanning Probe Microscopy

S. Kuriakose[1,2], F. Carrascosa[1], A. Castellanos-Gómez[1] and C. Munuera[1]

[1] *Instituto de Ciencia de Materiales de Madrid (ICMM-CSIC), c/ Sor Juana Inés de la Cruz, 3, Madrid, Spain*
[2] *CSIRO, Bradfield Road West Lindfield NSW 2070, Sydney, Australia*

Two-dimensional (2D) van der Waals materials have shown great potential for integration as components in electronic devices due to their unique electrical and optical properties [1]. Understanding the local behavior of these devices, often dominated by highly localized phenomena, is crucial for advancing in their application. Being ‘all surface’, this family of materials is particularly suited to be studied with local probe microscopy techniques and, taking a step further, within the device in its actual operational state [2-4]

In this talk, I discuss our recent approach to systematically study MoS_2-based devices under operando conditions, using Kelvin probe force microscopy (KPFM) to map the surface potential distribution of biased samples. Our primary focus has been on investigating the contact between the electrode and 2D material, which significantly impacts device functionality and efficiency by influencing charge injection into the semiconductor materials via the contact metal.

By employing a two-terminal configuration, we can effectively probe the voltage drops accross the device through surface potential mapping. Based on the choice of electrode material, our findings reveal the ohmic and Schottky behavior of the contact, offering insights for optimizing 2D-based devices such as highly rectifying diodes or transistors with low contact resistance.

This study aims to contribute to the advancement of 2D material-based electronics by providing valuable insights into the fundamental aspects of device operation and optimization strategies.

[1] Y. Liu, X. Duan, H. J. Shin. et al., Nature, 591 43 (2021).
[2] A. Behranginia, P. Yasaei, A. K. Majee et al., Small 13, 1604301 (2017)
[3] Y. Vaknin, R. Dagan and Y. Rosenwaks, Nanomaterials 10, 2346 (2020)
[4] M.A. Aslam, T. H. Tran, A. Supina, et al., npj 2D Mater. Appl. 6, 76 (2022).

I8

Nanomechanical probing, manipulation, and control of excitons in 2D materials

Kirill Bolotin

Institut für Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany

Mechanical strain can be used to manipulate material's symmetries. In this talk, we will i) demonstrate an approach to induce mechanical strain with controlled tensorial components in 2D materials at cryogenic temperatures and ii) use the strain response 2D semiconductors and heterostructures to study their excitons. First, we discuss the approaches toward mechanical strain engineering of high-quality suspended 2D material devices capable of inducing uniform or uniaxial strain with in-situ tunable magnitude and compatible with cryogenic measurements. Next, show that normally “dark” excitons with vanishing oscillator strength become observable in strained devices. Then, we discuss the approach to detect the valley character of intervalley excitons by examining their strain signatures. Finally, we show that the application of uniaxial strain leads to the behavior of the pseudospin degree of freedom that can be described in the language of the pseudomagnetic field. Such a pseudomagnetic field will be used to establish the many-body character of debated excitonic states.

I9

Exciton, charge and spin lattices in moiré heterostructures

Alexander Högele [1]

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Semiconductor van der Waals heterostructures with near-resonant band alignment and non-commensurate lattices such as MoSe2/MoTe2 [1] and MoSe2/WS2 [2] constitute peculiar model systems for excitons, charges and spins localized on moiré lattices. Being robust against mesoscopic lattice reconstruction [3] due to sizable lattice mismatch, they exhibit canonical periodic moiré potentials, while near-resonant band alignment induces hybridization of exciton states across the constituent layers. Using cryogenic optical spectroscopy of moiré excitons, we study the effects of correlated charge and spin ordering in such moiré heterostructures with different twist-angle configurations, highlighting emergent magnetism phenomena on effective monolayer and bilayer Hubbard triangular lattices [4]. Moreover, by employing open cavities, we establish control over neutral and charged moiré exciton-polaritons in the regime of strong light-matter coupling, thereby expanding the realm of moiré phenomena in van der Waals heterostacks.

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I10

Electrostatically defined quantum dots in bilayer graphene

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Graphene and bilayer graphene (BLG) are promising materials for quantum technologies. Considerable effort has been devoted to the study of quantum dot (QD) devices based on these materials. The main challenge in using graphene for such applications is the lack of a band gap, which prevents electrostatic confinement of electrons. A common solution has been to physically etch graphene to create hard wall confinement, but this method is hampered by edge disorder, making it difficult to make clean quantum devices.

In contrast, BLG can circumvent the edge disorder problem due to its tunable bandgap (up to 120meV) when subjected to a perpendicular electric field, enabling electrostatic soft confinement. This talk will present recent progress in gate-controlled single and double quantum dot operations in electrostatically gapped BLGs. The devices demonstrate a high degree of control, enabling gate-defined electron-hole and electron-electron double quantum dot systems with single electron occupancy. Few-electron/hole states have been achieved in the single dot regime, with excited state energies extracted and analyzed under parallel and perpendicular magnetic fields.

Recent data on ultra-clean BLG quantum dots will be presented, highlighting the study of spin-valley coupling, electron-hole crossover and symmetry between electron and hole states. In addition, findings on BLG quantum dots focusing on spin and valley lifetimes will be discussed. This work lays the foundation for the development of spin and valley qubits in graphene.

I11

Correlated kinetic magnetism of electrons in semiconductor moiré materials

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Since the discovery of magic-angle twisted bilayer graphene, moiré bilayers consisting of two monolayers of van der Waals materials have emerged as a highly-tunable platform for accessing novel correlated phases of matter. A small twist angle and/or a lattice mismatch between the constituting monolayers in these structures gives rise to a superlattice potential that breaks the electronic bands into a series of flat moiré minibands, which in turn sizably enhances the stability of correlated electronic phases. Recently, this approach has led to the observation of a plethora of exotic electronic states, ranging from Mott-Wigner crystals to fractional Chern insulators.

In this talk, I will describe our low-temperature spectroscopic experiments on magnetism of electrons in the vicinity of a Mott insulating state in angle-aligned, AA-stacked MoSe2/WS2 heterobilayer [1]. Owing to a strong, triangular moiré superlattice potential, the electrons forming a Mott state in such a structure are deeply localized within their moiré lattice sites, which renders their exchange interactions to be vanishingly small. However, as soon as the Mott state is doped with electrons that form doublons at already-occupied sites, the system begins to exhibit prominent ferromagnetic correlations, with the corresponding Curie-Weiss temperature being proportional to the number of doublons. As proven by our density-matrix-renormalization-group (DMRG) calculations, this ferromagnetism is not driven by inter-electron exchange interactions, but by the minimization of the kinetic energy of doublons through the Nagaoka mechanism. Such a kinetic origin of ferromagnetic correlations in our system is further confirmed a sizable drop in critical temperature that we observe at 4/3 filling factor of the moiré lattice, where the doublons form a Mott-Wigner state in which their mobility is strongly suppressed. These observations constitute a direct evidence for kinetic Nagaoka magnetism in an extended, two-dimensional system.

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I12

Controlling Spins using Chiral 2D Perovskite Semiconductors

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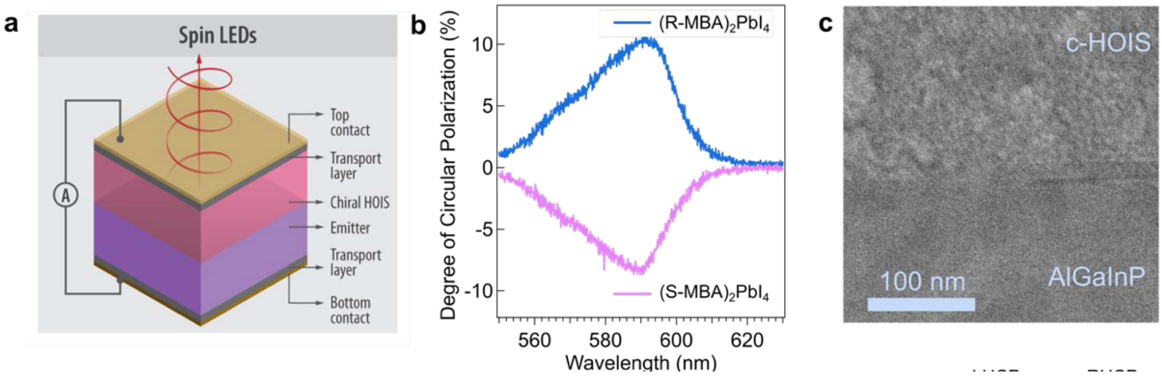
Chiral hybrid organic-inorganic perovskite semiconductors (c-HOIS) combine the unique and functional aspects of inorganic semiconductors with chiral molecules. The inorganic semiconductor borrows the chirality of the organic component to yield a unique family of highly tunable chiral semiconductors. Semiconductors already form the backbone of mdern-day technologies adding chirality and control over spin through CISS provides new avenues for creative technological development. The family of c-HOIS that we are disussing here consists of a framework of metal-halide polyhedra spaced by non-coordinating chiral organic cations. Here, we demonstrate spin injection across chiral halide perovskite/III-V interfaces achieving spin accumulation in a standard semiconductor III-V $(Al_xGa_{1-x})_{0.5}In_{0.5}P$ multiple quantum well (MQW) light emitting diode (LED). The spin accumulation in the MQW is detected via emission of circularly polarized light with a degree of polarization of up to ~15%. The chiral perovskite/III-V interface was characterized with X-ray photoemission spectroscopy (XPS), cross sectional scanning Kelvin probe force microscopy, and cross section transmission electron microscopy (TEM) imaging, showing a clean semiconductor/semiconductor interface where the fermi-level can equilibrate. These findings demonstrate chiral perovskite semiconductors can transform well-developed semiconductor platforms to ones that can also control spin.



I13

Controlling Excitons in van-der-Waals materials in tunable optical cavities

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Two dimensional materials have emerged as a new and interesting platform for studies of tightly bound exciton in ultimately thin materials. Meanwhile, various types of 2D- or quasi 2D materials have become available that feature giant light-matter interactions, charge tunability, and intriguing magnetic and topological properties. These features can all be exploited for implementing novel photonic devices, and for fundamental, as well as quantum photonic investigations in the framework of cavity quantum electrodynamics [1].

I will discuss the implementation of open optical cavities in liquid helium free optical cryostats [2], which are ideally suited for the study of exciton-polaritons using 2D materials. I will address examples of such experiments, including cavity-controlled temporal dynamics of trapped excitons in the weak coupling regime, the magnetic properties of charge-correlated exciton-polaritons in the regime of strong light-matter interaction and give perspectives towards polaritonics at telecommunication wavelength.

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I14

Moiré Minibands, twist disorder and exciton-phonon coupling in van der Waals stacks

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Two-dimensional (2D) materials are atomically thin crystals characterized by strong in-plane chemical bonds and weak van der Waals (vdW) coupling between adjacent layers allowing to assemble vdW stacks. Heterobilayers of transition-metal dichalcogenides such as MoSe2/WSe2 host dense ensembles of interlayer excitons potentially forming a coherent many-body state at low temperature [1-2]. Moreover, twisted homobilayers such as tWSe2 are prone to the formation of moiré minibands.

Here, we approach the electron-phonon coupling as well as collective electronic excitations in those atomically thin crystals by means of low-temperature resonant inelastic light scattering (RILS) spectroscopy. RILS is a well-established powerful method to study low-dimensional interacting electronic systems [3] as well as (exotic) correlated phases [4]. In tWSe2 bilayers, we access a series of RILS modes showing a peculiar dependence on twist angle and temperature that are interpreted as single-particle like collective inter-moiré-band excitations (IMBE) [5]. These observations allow to quantitatively probe the formation of a series of moiré-bands and demonstrate the potential to study correlated electron phases in twisted bilayers.

We gratefully acknowledge financial support by the DFG via the SPP 2244 and grants WU 637/4-2, 7-1.

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I15

Hybrid Organic-Inorganic 2D Materials

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Hybrid organic-inorganic 2D materials – including 2D halide perovskites and metal organochalcogenolates (MOCs) – are chemically tunable excitonic semiconductors with applications ranging from solar cells to light-emitting devices to photonic circuits to quantum information. In these emerging materials, the combination of quantum and dielectric confinement, strong exciton-phonon coupling, and dimensionality reduction offer unprecedented opportunities for controlling light-matter-charge interactions through chemistry. In this talk, I will describe recent work from my lab on the synthesis of hybrid semiconductor nanomaterials and our evolving understanding of how structure and chemical functionalization influence excited state dynamics. Using a combination of ultrafast laser spectroscopy, timeresolved optical microscopy, and kinetic modeling, we will explore the impact of nonequilibrium population dynamics on excited state transport phenomena and the emergence of unique electronic and vibrational phenomena.

I16

Manipulation and transport of excitons in 2D semiconductors and antiferromagnets

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Two-dimensional transition metal dichalcogenides offer an excellent platform to study non-linear dynamics of tightly-bound exciton quasiparticles. The properties of the excitons and their optical response change drastically in the presence of free charges, leading to emergence of many-body states described as trions or Fermi polarons. The physics of such Bose-Fermi quasiparticle mixtures have attracted a lot of interest in the scientific community and motivated the development of methods to control them on ultrafast time-scales. In addition, excitons were recently demonstrated to play central role also for magnetic 2D materials, with open questions regarding exciton mobility and its relation to the magnetic order, from both fundamental and technological perspectives.

The first part of the talk will be focused on the use of intense THz pulses to transiently modify light-emission of exciton-electron ensembles in monolayer semiconductors. We demonstrate a near complete, THz-induced trion-to-exciton conversion by monitoring time resolved photoluminescence after optical excitation. It offers new pathways to manipulate exciton-electron mixtures, triggering a non-linear optical response by low-energy photons on picosecond timescales. In the second part, I will discuss exciton transport in the layered semiconducting antiferromagnet CrSBr. Strong influence of the magnetic order on the exciton propagation will be discussed including rapid, non-linear exciton expansion in ultra-thin layers as well as contraction of the exciton clouds at low temperatures. These results are particularly interesting in the context of magnetic control of exciton transport and the consequences of coupling optical excitations to the magnetic order.

I17

Low-dimensional halide perovskite emitters – Accelerated discovery and enhanced optical protperties

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To meet the current and future global energy demands, we must implement a dual strategy of increased renewable energy conversion and reduced energy consumption. This will require us to substantially optimize current materials or discover and develop entirely new ones, for example, for solar cells and light-emitting diodes. A material with vast potential for these applications is nanocrystalline halide perovskite. However, one of the difficulties in improving perovskites is that the fabrication can be too fast to investigate with conventional approaches, and optimizing the resulting NCs can be an extremely tedious task. In this talk, I will discuss our new multimodal approaches to determine the structure and synthesis dynamics of highly confined 1D and 2D halide perovskite nanocrystals, tailor them to specific applications, and enhance their efficiency and stability.[1,2,3] I will also highlight our approach to incorporate a machine-learning process to optimize syntheses with minimal data demand. Importantly, many of these novel approaches can readily be applied to other systems, greatly benefitting material discovery and development.

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I18

Quantum Emitters in van der Waals layered materials

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The exceptional optical properties of quantum defects in van der Waals layered materials, particularly in the context of spin-photon interfaces, have generated significant interest. These 2D semiconductors, which are only a few atoms thick, offer high light transparency and structural openness, overcoming challenges related to photon extraction. The unscreened nature of defects in these ultrathin layers leads to deeper and more confined defect states, which are well-separated from band edges, making it easier to establish a two-level quantum system. However, creating quantum defects deterministically remains a major challenge. The ability to engineer these defects at the nanoscale is crucial for large-scale quantum photonics. In a recent study, we discussed our work on generating quantum defects in hexagonal boron nitride (hBN) flakes using a controlled femtosecond laser pulse process with a threshold tracking method. This technique results in a near-unity yield of high-quality quantum emitters at each laser-processed site, with largely suppressed background emission. Under continuous-wave excitation, the quantum emitters exhibit stable single-photon count rates of more than 10 Mcts/s at saturation, with negligible spectral diffusion. These results demonstrate the possibility of deterministically generating optically active color centers with a few nanometer resolutions via femtosecond laser pulse writing. This achievement offers a powerful tool for engineering quantum photonic chips, opening new avenues for quantum technologies to revolutionize various fields.

I19

Xenes – chemistry beyond graphene

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The Xenes is group of monoelemental two dimensional materials. Beyond the graphene, first material prepared in monolayer form, many others were reported in last two decades. The most explored group of monoelemental 2D materials are tetrel, the 14th group of elements (C, Si, Ge, Sn, Pb) and pnictogens belonging to 15th group of elements (N, P, As, Sb, Bi). Beyond these several other monolayers of p-block elements like borophene and tellurene as well as metal layers like goldene or molybdene.

The strategies for the synthesis of the Xenes from tetrel and pnictogen group of elements will be described. Compare to the pnictogens, where the elements posses layered structure, the tetrel need to be prepared in layered form using different strategy. The chemical exfoliation of layered compounds containing tetrel layers are chemically exfoliated in order to obtained this group of 2D materials. The different strategies applied for synthesis of different Xenes as well as their exfoliation methods will be discussed.

The chemistry of Xenes is extremely variable and different strategies are applied for mechanically and chemically exfoliated materials. The covalent and non-covalent functionalization of will be described for the pnictogen group and differences in chemistry of these elements, especially transition from phosphorus to arsenic. The tetrel functionalization usually procced already during their chemical exfoliation. Thanks to effective formation of bods between carbon and silicon/germanium as well as many other elements, high degree of functionalization is possible to reach up to complete stochiometric coverage. Variability in surface functionalization allowed broad spectra of application in filed of energy storage, electronic, sensing and many others. [1]

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I20

Quantum Functionality in 2D materials: From Moiré Structures to Quantum Confined Devices

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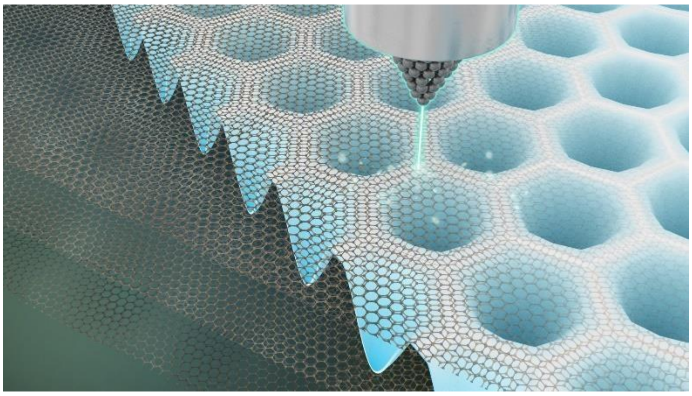
Material systems, devices, and circuits, based on the manipulation of individual charges, spins, and photons in solid-state platforms are key for quantum technologies. The field of twodimensional (2D) materials presents an emerging opportunity for the development of nextgeneration quantum technologies, while also pushing the boundaries of fundamental understanding of condensed matter systems.

Through a combination of nanofabrication methods, scanning probe microscopy, and other supporting techniques, our laboratory explores quantum functionality in 2D materials and their heterostructures.

In the first part of the talk, I will focus on novel phenomena in moiré structures created by twisting 2D layers. I will discuss the demonstration of reversible local response of domain wall networks using scanning tunneling microscopy in ferroelectric interfaces of marginally twisted WS_2 bilayers. Moreover, in the case of twisted WS_2 bilayers close to 60°, we observe signatures of flat bands and study the influence of atomic relaxation on their band structure. In the second part of the talk, I will discuss our progress in realizing quantum-confined devices in 2D semiconductors, including quantum dots and quantum point contacts.



I21

Magneto-optical properties in the vdWs $NiPS_3/WSe_2$ heterostructure

Adi Harchol [1], Shahar Zuri[1], Kusha Sharma[1], Elenor Gerrafy[1], Rajesh[2], D. Naveh[2], T. Brumme[3], T. Heine[3] and E. Lifshitz[1]

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The recent interest in magnetic two-dimensional (2D) van der Waals (vdW) materials changed paradigms in science and technology, endowing intriguing possibilities in controlling magnetism via external stimuli, like strain, electric field or proximity effect. The current study addressed vdW heterostructures (HSs) comprising layers of MPX_3 (M-metal, X-chalcogen) antiferromagnets (AFM) with non-magnetic transition metal dichalcogenide (TMDC) layers, focusing on tunning of magneto-optical properties of the AFM layers under the proximity of another layer, using the micro-photoluminescence (μ-PL) spectroscopy. Representative μ-PL spectra of the pristine NiPS3 (blue line) and the related HS (red line), recorded at 4K, are shown in Figure 1a, revealing a spectral shift from one other. The could be attributed to the influence of WSe_2's proximity on the $NiPS_3$ layer, by altering the dielectric environment around it. The μ-PL spectra of the exposed $NiPS_3$ area, as well as at a few spots across the HS, were recorded at various temperatures and under a gradual increase of the strength of an external static magnetic field up to ±8 Tesla. The degree of linear polarization (DLP) varied from ~ 32% in the pristine $NiPS_3$ to a higher value of 70% in the HS under a field with +8 Tesla (not shown here). Most interestingly, $NiPS_3/WSe_2$ HS also exhibits a unique circular polarization. Representative scans of the HS's PL, recorded under the influence of an external magnetic field and monitored by two opposing circular polarizations, are shown in Figure 1b. This set of spectra depicts a net polarization of ~ 80% at 0 Tesla that disappeared at +8 Tesla, however, it is nearly fully maintained up to -8 Tesla. In addition, the plot of the degree of circular polarization versus the strength of the magnetic field (not shown here), uncovers a nonlinear behavior at low magnetic fields. The indicated observation proposed the existence of a Rashba effect. Currently, we are assuming that such an effect is induced by the SOC of the heavy W-atoms, in proximity to the $NiPS_3$ magnetic layer. Alternatively, the effect can be associated with an interaction between W(d) and Ni(d) orbitals in proximate layers along the stacking direction. We excluded a major strain effect from a substrate of cladding via control experiments (not shown here), we assume that our observations are related to mutual influences of layers within the HS. The study is currently corroborated by a theoretical model, for verifying the mechanism that induces the unique chirality to the HS.

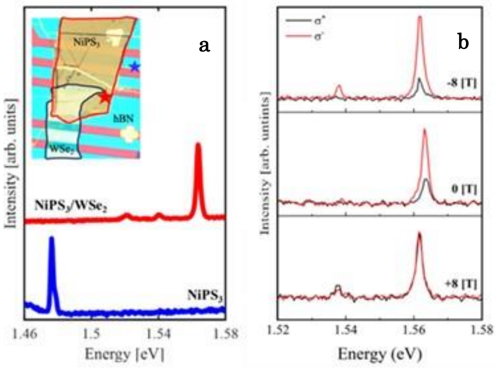

Figure 1: ***Magneto-optical properties of*** $NiPS_3/WSe_2$: ***a****. Comparison between the PL spectra of barred* $NiPS_3$ *(blue line) and* $NiPS_3/WSe_2$ *HS (red line). The inset shows an optical image of the HS device;* ***b****. The PL spectra of the HS were monitored through circular polarizers (see indent) and under the influence of an external magnetic field (the strength in units of Tesla).*

I22

Data-driven discovery of novel 2D materials

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The field of 2D materials has evolved with tremendous pace over the past decade and is currently impacting many contemporary subfields of physics including spintronics, valleytronics, unconventional superconductivity, multiferroics, and quantum technologies. Vertical stacking of 2D materials offers unique opportunities for creating designer structures with novel properties absent in the constituent monolayers with the emergence of superconducting phases in twisted bilayer graphene being a particularly striking example. Unfortunately, experimental advancements beyond the proof-of-principle level are impeded by the vast size of the configuration space defined by layer combinations and stacking orders. In this talk I will show how automated density functional theory (DFT)-based workflows can be combined with deep generative models to systematically create novel monolayer structures and characterize their physical properties [1,2]. Following such approach we have characterized more than 15000 monolayers and made the results available in the open C2DB database [3]. Recently, we have stacked the 1000 most stable monolayers in all possible (non-twisted) stacking configurations and validated the structures by comparing to experiments [4]. We identify an abundance of bilayers that support two or more (meta)stable stackings with different magnetic or electrical properties making them candidates for the emerging field of slidetronics. If time permits, I will discuss our efforts to discover and design novel point defects in 2D insulators for quantum technology applications [5,6].

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I23

Everything you always wanted to know about bilayers

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One subclass of 2D materials are bilayers of 2D crystals. This subclass has found a lot of attention after the discovery of flat bands and correlated phases in bilayer graphene, but interesting phenomena have already been reported earlier, e.g. the direct to indirect band gap transition when going from mono- to bilayer in various transition metal dichalcogenides.

As the interlayer interaction is governed by London dispersion, it is not obvious why the electronic structure of the bilayer can differ so strongly from that of the monolayers. From a pragmatic viewpoint, the interlayer distance has a strong impact on the electronic structure of the bilayer, and requires an accurate assessment by theory. Unfortunately, density-functional theory (DFT) is notoriously erroneous for this type of interaction, and requires special attention.

In this lecture I will first discuss the different ways of stacking 2D crystals. For buckled honeycomb lattices that are known for group 13-15 2D crystals I will propose a unique nomenclature that facilitates communication and allows to identify all high-symmetry bilayer configurations [1,2].

I will further elaborate on accurate calculations of interlayer energies for various 2D materials and comment on the performance of DFT on these systems [3,4]. Finally, I will discuss typical models for the description of van der Waals heterostructures of 2D crystals and highlight that different models should be utilized when describing 2D crystals prepared by direct growth or by transfer methods. The impact on twisted bilayer MoS_2 will be highlighted in detail [5].

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I24

Photon upconversion in monolayer transition metal dichalcogenides

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The monolayer transition metal dichalcogenides (TMDs) emerge as an outstanding platform to study electron- electron and electron- phonon interaction [1-4]. Their two-dimensional (2D) nature and the reduced dielectric screening of the Coulomb interaction allow for the formation of excitons with a binding energy of hundreds of meV and high-order excitonic complexes, such as trions and biexcitons with binding energies of tens of meV. Moreover, due to the strong spin- orbit coupling in TMDC monolayers and the resulting valley-contrasting spin splitting at the K valleys, the excitonic complexes possess both the spin as well as valley degree of freedom.

In optically darkish systems, such as WS_2 and WSe_2 monolayers, the electric- dipole forbidden (optically dark) exciton state is positioned at lower energy than the optically active exciton state. On the contrary, in $MoSe_2$ monolayers the bright exciton state is at the lowest energy. These level hierarchies as well as exciton- phonon interactions were studied due to the progress in elaborating high-quality hBN-encapsulated TMDC monolayers. In this context, upconversion (UPC) photoluminescence (PL) spectroscopy recently provided thorough insights into exciton- exciton and exciton- phonon interactions and was successfully employed to reveal the coupling between various excitonic complexes in the optically darkish and bright hBN-encapsulated TMDs monolayers. In particular, upconversion of light from dark excitons [2], trions [1-4], and biexcitons to bright excitons was observed [3-4].

In my talk, I will provide an overview of upconversion PL processes in monolayer TMDs and their van der Waals heterostructures.

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I25

Spontaneous photovoltaic effect in polar 2D materials

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One of the distinct characteristics of 2D materials is their exceptional susceptibility to symmetry manipulations. Techniques such as application of strain, stacking with desired alignment, and surface functionalization can alter their symmetry, offering an attractive platform to explore intrinsic photovoltaic effects which are highly dependent on the material's symmetry. This is evidenced by the recent findings demonstrating an enhanced bulk photovoltaic effect in aligned van der Waals heterostructures and depolarization-field-induced photovoltaic effect in rhombohedrally stacked MoS_2. These discoveries not only pave the way for novel optoelectronic devices with customized photoresponses but also open avenues for exploring fundamental condensed matter phenomena, utilizing symmetry-engineered 2D materials. In this talk, I will present our recent research on identifying various mechanisms behind the spontaneous photovoltaic effect in 2D semiconductors with induced and spontaneous polarization. Further, I will discuss the relevance and application of conventional theories to heterostructure systems.

I26

3D Integration of 2D Devices for Advanced Memory, Logic, and Bio-inspired Computing

Saptarshi Das, PhD.

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Electrical Engineering and Computer Science, Materials Science and Engineering,

Materials Research Institute, Pennsylvania State University, University Park, PA, USA

Abstract: In this presentation, I will delve into the exciting realm of monolithic 3D integration, where emerging 2D FETs take center stage, empowering advanced memory, and logic devices. Notably, our recent breakthroughs have culminated in the successful demonstration of wafer-scale 2-tier and 3-tier 3D integration, utilizing MoS_2 and WSe_2 FETs as the building blocks. These achievements have paved the way for multifunctional circuits that hold immense promise for the future of electronics. Furthermore, I will also discuss our work on bio-inspired neuromorphic computing. We have harnessed the potential of 2D materials to design solid-state devices with low power consumption mimicking auditory processing in barn owl, collision avoidance in locust, probabilistic computing in dragonfly, and multisensory integration in octopus. By combining the power of 2D materials with bio-inspired principles, our work lays a solid foundation for the creation of highly compact and functionally diverse integrated circuits in the revolutionary third dimension. The implications of this technology are far-reaching and hold the potential to shape the future of electronics and computing.

Biography: Dr. Das received his B.Eng. degree (2007) in Electronics and Telecommunication Engineering from Jadavpur University, India, and Ph.D. degree (2013) in Electrical and Computer Engineering from Purdue University. He was a Postdoctoral Research Scholar (2013-2015) and Assistant Research Scientist (2015-2016) at Argonne National Laboratory (ANL). Dr. Das joined the Department of Engineering Science and Mechanics (ESM) at Penn State University in January 2016. Dr. Das was the recipient of Young Investigator Award from United States Air Force Office of Scientific Research in 2017 and National Science Foundation (NSF) CAREER award in 2021. Das Research Group at Penn State focuses on 2D microelectronics for bio-inspired sensing, neuromorphic computing, and hardware security.

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I27

Exciton Manipulation and Transport in 2D Semiconductor Heterostructures

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*Equal contribution

Long-lived interlayer excitons in van der Waals heterostructures based on TMDCs have recently emerged as a promising platform for controlling exciton transport on the mesoscopic length scales, allowing control over exciton diffusion length, energy and polarization. One of the driving forces for exciton transport is the interaction between out-of-plane dipoles in the exciton bosonic gas. By using spatial and time-resolved photoluminescence imaging, we can observe the dynamics of exciton transport, enabling a direct estimation of the exciton mobility [1]. The presence of interactions significantly modifies the diffusive transport of excitons, effectively acting as a source of drift force and enhancing the diffusion coefficient by one order of magnitude. In certain types of vdW heterostructures, the layer hybridization and exciton-exciton interaction can also be electrically tuned, allowing us to uncover dipole-dependent properties and transport of excitons with different degrees of hybridization [2]. Moreover, we find constant emission quantum yields of the transporting species as a function of excitation power with dominating radiative decay mechanisms dominating over nonradiative ones, a fundamental requirement for efficient excitonic devices.

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I28

Strain engineering phase transition in $NbSe_2$

Eudomar Henríquez-Guerra [1], Hao Li [2], M Reyes Calvo [1], Andres Castellanos-Gomez [2]

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In recent decades, researchers have explored diverse avenues to manipulate the critical temperature (Tc) —the temperature at which materials transition to the superconducting state. Techniques ranging from light irradiation to electrostatic doping have been employed in efforts to modulate Tc and unlock new frontiers in superconductivity. Notably, pressure and strain represent particularly powerful tools in this pursuit, offering direct control over material properties at the atomic level. Among the materials investigated, niobium diselenide ($NbSe_2$) have emerged as promising platforms for exploring superconductivity under pressure and strain. Previous studies have primarily focused on the effects of uniaxial strain or hydrostatic pressure on bulk crystals, revealing intriguing modifications in Tc and electronic structure. However, investigations into biaxial strain effects and thin flakes of $NbSe_2$ remain limited, despite their potential for more efficient strain transfer and enhanced tunability.

In this talk, we will discuss strain engineering in $NbSe_2$ nanosheets, aiming to fill the gap in our understanding of biaxial strain effects on superconductivity. By exploring thin $NbSe_2$ flakes, we seek to elucidate the intricate interplay between strain, electronic structure, and superconducting properties. Our findings not only contribute to the fundamental understanding of superconductivity in two-dimensional materials but also pave the way for practical applications harnessing strain as a versatile tool for tailoring material functionalities.

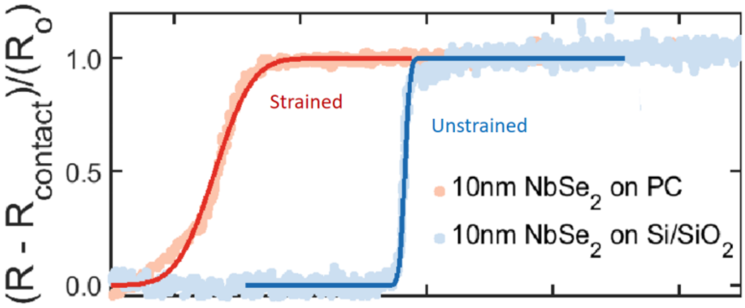

Figure 1. Resistance vs. temperature measured on two samples of 10 nm thick $NbSe_2$, one made on Si/SiO_2 (unstrained) and one made onto polycarbonate (biaxially compressed ~1.1%)

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I29

Modulation of Ultrafast Quasiparticle Dynamics in Two-dimensional Semiconductors

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In single-layer semiconducting transition metal dichalcogenides (TMDs), strong quantum confinement and reduced dielectric screening, due to their two-dimensional structure, leads to tightly bound excitons, trions and higher-order bound states. Understanding the temporal evolution of such complexes after optical excitation and their response to external stimuli is essential for unlocking their potential in optoelectronic applications.

First, we investigate the influence of electrostatic doping via the field-effect on the ultrafast dynamics of trions in single-layer TMDs using broadband femtosecond pump-probe microscopy. We study the temporal dynamics of excitons and trions as the primary photoexcited species, disentangle the formation of trions from photogenerated vs electrostatically injected charge carriers and discuss the formation of neutral and charged biexcitons.

As a second control parameter, we apply uniaxial strain and observe a modulation of the exciton and charge carrier dynamics via a change in their mobility and interaction with trap sites.

Flatlands

Contributed presentations

C1

Wafer-scale Hexagonal Boron Nitride for Hydrogen Generation by Radiolysis of Interfacial Water

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Hydrogen is an important building block in global strategies toward a future green energy system. To make this transition possible, intense scientific efforts are needed, also in the field of materials science. Hexagonal boron nitride (h-BN) is a very promising candidate for such applications, as it has been demonstrated that micrometer-sized flakes are excellent barriers to molecular hydrogen. However, it remains an open question whether large-area layers fabricated by industrially relevant methods preserve such promising properties. We address this issue and show results on the growth of epitaxial h-BN on 2 inch sapphire wafers by metalorganic vapourphase epitaxy (MOVPE) [1-5], which is currently regarded as one of the most promising growth techniques. This technique allows to grow uniform hBN layers [2,3], which can also serve as a substrate for the direct growth of van der Waals heterostructures on the wafer-scale [5]. In this work, we show that electron-beam-induced splitting of water creates hBN bubbles (Fig. 1) that effectively store molecular hydrogen for weeks [1]. The bubble formation can be observed in-situ in a scanning electron microscope, giving us the unique possibility to visualize the hydrogen generation process. Raman spectroscopy proves the presence of molecular hydrogen and experiments with heavy water provide evidence that hydrogen generation is triggered by the radiolysis of water captured at the van der Waals interface. By performing a stress test we could also demonstrate that H_2 remains in the bubble even after extreme wear and deformation, highlighting the suitability of our large-area epitaxial material for possible hydrogen storage applications.

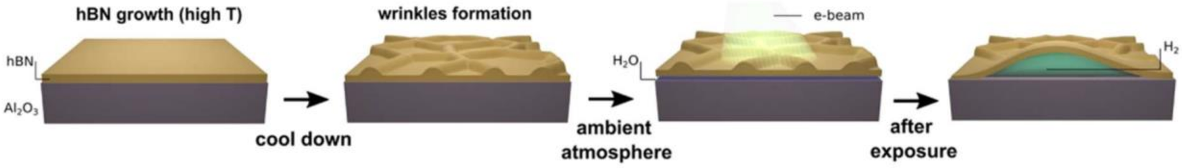

Fig. 1: Schematic illustration of the bubble formation. hBN is grown by MOVPE at temperatures above 1000 °C. After the growth the sample is cooled to room temperature, which leads to the formation of hBN wrinkles. The sample is removed from the reactor and exposed to ambient conditions. Electron beam exposure in an SEM leads to bubble formation [1].

Our findings show that epitaxial h-BN by MOVPE is not only a potential candidate for hydrogen storage, but also holds promise for the development of unconventional hydrogen production schemes.

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Ion Transport Dynamics in Single MXene Nanoparticles Revealed by Interferometric Scattering Microscopy

<u>Mohsen Beladi Mousavi</u>,[1] Franz Gröbmeyer,[1] Christoph Gruber,[1] Kyle Matthews,[2] Kateryna Shevchuk,[2] Alex Inman,[2] John Wang,[2] Yury Gogotsi,[2] Emiliano Cortes[1]

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"MXene, a novel class of two-dimensional materials, holds significant potential in revolutionizing energy storage systems due to its exceptional electrical conductivity, large surface area, and ability to accommodate various ions, enhancing the performance of batteries and supercapacitors.[1-2] In this pioneering study, state-of-the-art operando microscopy, *i.e.*, interferometric scattering microcopy (iSCAT) reveals the intricacies of ion diffusion within MXene nanostructures at the scale of individual nanoparticles (Fig. 1). The research delivers an in-depth analysis of the dynamics of ion transport and charge transfer, shaped by variables such as ion size, hydrophilicity, and the nature of the solvent used. The deployment of non-invasive operando microscopy for live tracking has shed light on the influence of these variables on ion mobility within MXene frameworks. Notably, the research has identified how ion diffusion contributes to power density at the nanoparticle level, thus enhancing our ability to precisely measure the boundaries of charge transport in MXene films. These breakthroughs are vital for the advancement of energy storage technologies, providing a clearer understanding of ion movement at the nanoscale and its implications for the efficacy of high-performance materials. This investigation lays the groundwork for future enhancements in energy storage devices, suggesting that fine-tuning ion transport could markedly elevate power density and efficiency."

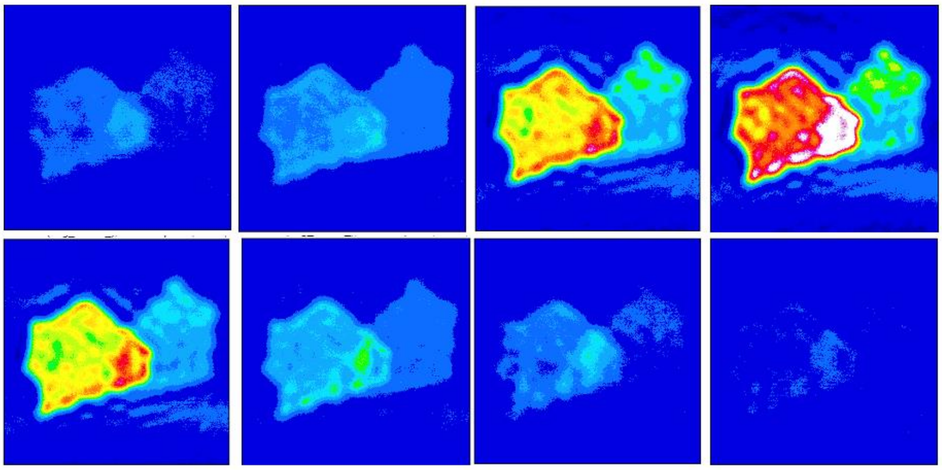

Fig. 1. Progressive stages of ion diffusion in a single MXene nanoparticle observed under operando conditions, depicted in a sequence from left to right.

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C3

Collosal field-induced energy shift of higher-energy excitons in CrSBr

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CrSBr was quite recently recognized as an interesting platform combining magnetic ordering and good optical properties. This semiconductor exhibits strongly anisotropic direct-band gap excitations in the near-infrared energy range [1]. Showcasing the intriguing coupling of electronic and magnetic properties, the energy of an exciton was shown to be affected by the magnetic interlayer ordering.

The standard exciton states with energy around 1.32 eV have been thoroughly examined for their prominent tunability in magnetic field of around 15 meV. In this work we present observation of higher-bands exciton states in the same material. With identical anisotropy and qualitatively analogous field dependence, the reported states offer over 7 times wider span of field-tunable exciton energies. We present a phenomenological model of magnetic field-assisted coupling between two higher energy states fits to the extracted energies of the states, providing some insights into the surprisingly large energy shift observed when applying a magnetic field.

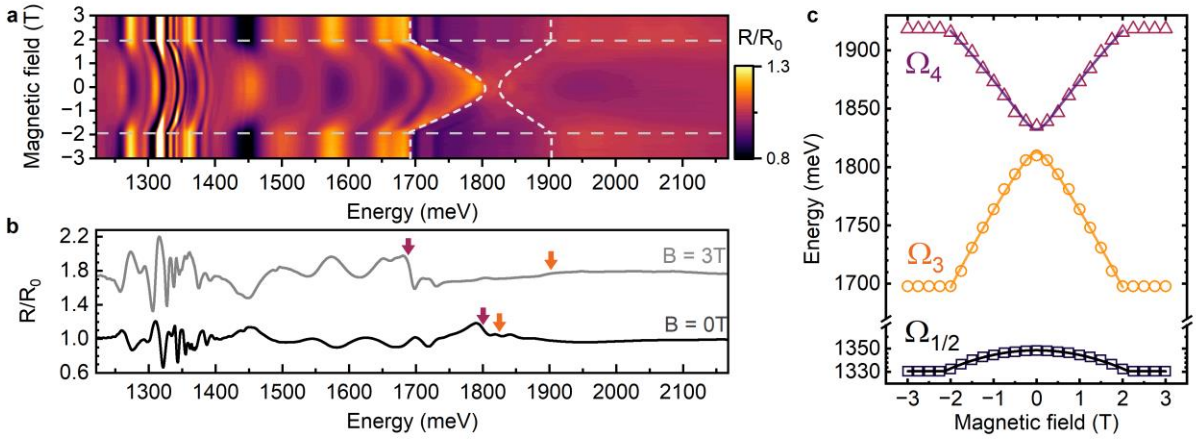

Fig. 1. a, Magnetoreflectance map normalized to the substrate reference in a wide energy range showcasing absorption of both the fundamental (1.3 eV) and the higher-bands (1.8 eV) exciton states. b, Comparison of extracted reflectance profiles in magnetic fields of 0T and 3T with two chosen higher-bands states highlighted with arrows. c, Extracted energies of earlier denoted states.

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C4

Laser-induced ultrafast spin injection in all-semiconductor magnetic CrI_3/WSe_2 heterobilayer

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Spin injection stands out as a crucial method employed for initializing, manipulating, and measuring the spin state of electrons, which are fundamental to the creation of qubits in quantum computing. However, ensuring efficient spin injection while maintaining compatibility with standard semiconductor processing techniques is a significant challenge. Herein, we demonstrate the capability of inducing an ultrafast spin injection into a WSe_2 layer from a magnetic CrI_3 layer on a femtosecond time scale, achieved through real-time time-dependent density functional theory calculations upon a laser pulse.[1] Following the peak of the magnetic moment in the CrI_3 sublayer, the magnetic moment of the WSe_2 layer reaches a maximum of 0.89 μ_B (per unit cell containing 4 WSe_2 and 1 CrI_3 units). During the spin dynamic, spin-polarized excited electrons transfer from the WSe_2 layer to the CrI_3 layer via a typeII band alignment. The large spin splitting in conduction bands and the difference in the number of spin-polarized local unoccupied states available in the CrI_3 layer lead to a net spin in the WSe_2 layer. Furthermore, we confirmed that the number of available states, the spin-flip process, and the laser pulse parameters play important roles during the spin injection process. This work highlights the dynamic and rapid nature of spin manipulation in layered all-semiconductor systems, offering significant implications for the development and enhancement of quantum information processing technologies.

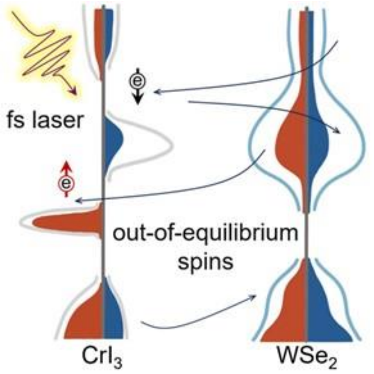

Figure 1: Schematic of spin injection in CrI_3/WSe_2 heterobilayer.

References [1] Guo, Y.; Zhang, Y.; Liu, Q.; Zhou, Z.; He, J.; Yuan, S.; Heine, T.; Wang, J. Laserinduced ultrafast spin injection in all-semiconductor magnetic CrI3/WSe2 heterobilayer. 2024, ACS Nano Article ASAP DOI: 10.1021/acsnano.3c12926.

C5

Strong Dipolar Repulsion of One-Dimensional Interfacial Excitons in Monolayer Lateral Heterojunctions

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Repulsive and long-range exciton−exciton interactions are crucial for the exploration of 1D correlated quantum phases in the solid state. However, the experimental realization of nanoscale confinement of a 1D dipolar exciton has thus far been limited. Here,[1] we demonstrate atomically precise lateral heterojunctions based at transitional-metal dichalcogenides (TMDCs) as a platform for 1D dipolar excitons. The electronic properties of a type II WSe_2−$WS_{1.16}Se_{0.84}$ lateral heterostructure were simulated and compared to the experimental data. The expansion of the exciton cloud driven by dipolar repulsion was found to be strongly density dependent and highly anisotropic. The interaction strength between the 1D excitons was experimentally determined to be $\sim 3.9 \times 10^{-14}$ eV cm^{-2}, corresponding to a dipolar length of 310 nm, which is a factor of 2−3 larger than the interlayer excitons at two-dimensional van der Waals vertical interfaces. These results suggest 1D dipolar excitons with large static in-plane dipole moments in lateral TMDC heterojunctions as an exciting system for investigating quantum many-body physics.

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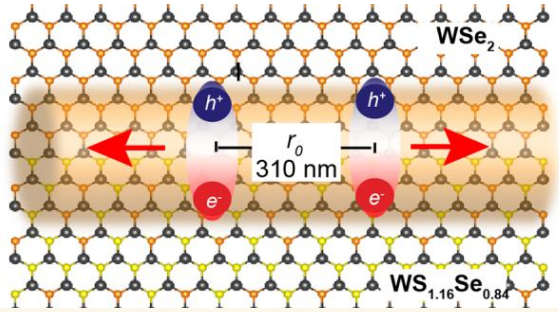

C6

Understanding the Impact of Non-Uniform Strain Fields on Exciton Dynamics in Multilayered 2D Transition Metal Dichalcogenides

M. Daqiqshirazi, T. Brumme

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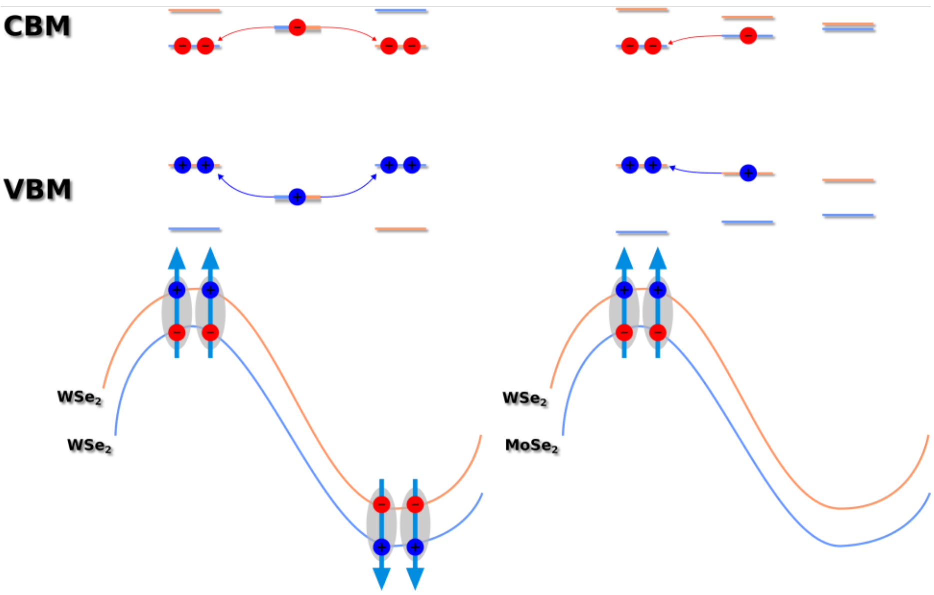
Full control of excitons in 2D materials is an important step towards using them in potential applications. Straintronics is one method that can be used to effectively control the movement of excitons. Unfortunately, the effects of non-uniform strain in 2D materials are not yet well understood theoretically, although these strain fields can be present in experiments in the form of wrinkles, bubbles, and folds, or even explicitly applied to 2D materials through pre-patterned surfaces. The effects of these non-uniform strain fields on multilayers are even less studied due to the sheer size of these systems. In the present investigation, we extend our study of monolayer wrinkles [1] to homo- and heterobilayers of 2D transition metal dichalcogenides using density functional theory. We show that the nonuniform strain leads to the formation of interlayer excitons in homobilayers of WSe_2 and to exciton localization in heterobilayers of WSe_2-$MoSe_2$. Our results also show that the brightening of the excitonic states under strain is related to a changed total angular momentum due to mixing of in- and out-of-plane states. Our results will pave the way towards a full understanding of the strain-control of excitons in 2D materials.

[1] M. Daqiqshirazi and T. Brumme, *Phys. Rev. B.* **108**, 155304 (2023).



Behavior of excited charge carriers in (left) bilayer WSe_2 and (right) heterobilayers of WSe_2 on $MoSe_2$. Due to the inversion symmetry in homobilayers the excited electrons and holes move to both high-strain regions but in heterobilayers they move towards the $MoSe_2$ part with the highest strain. In homobilayers the formation of interlayer exciton (as shown) is possible after a critical strain, possibly resulting in longer lifetimes.

C7

Tunable strain and bandgap in subcritical-sized MoS_2 nanobubbles

M. Gastaldo [1], **J. Varillas** [1,2], **A. Rodríguez** [3], **M. Velický** [1], **O. Frank** [1] **and M. Kalbáč** [1]

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In the exfoliation and transfer of 2D materials, nanobubbles naturally form at the interface between the 2D material and the substrate because of trapped contaminants. Nanobubbles are known to act as exciton recombination centers because of their reduced bandgap which is due to local strain. The strain, in turn, scales with the aspect ratio of the bubbles. The common understanding suggests that the aspect ratio is a universal constant independent of the bubble size [1]. In our work [2], by combining scanning tunneling microscopy measurements and molecular dynamics simulations, we show that the universal aspect ratio breaks down in MoS_2 nanobubbles below a critical radius ($R \approx 10$ nm). In this size range, the bending rigidity causes the aspect ratio to increase with increasing size [3]. Accordingly, atomic-level analysis indicates that the strain increases from 3% to 6% in the sub-critical size range. Using scanning tunneling spectroscopy, we further demonstrate that the bandgap decreases as a function of the size. Our results indicate that, by controlling the radius of the nanobubbles, tunable emitters may be obtained in 2D semiconductors.

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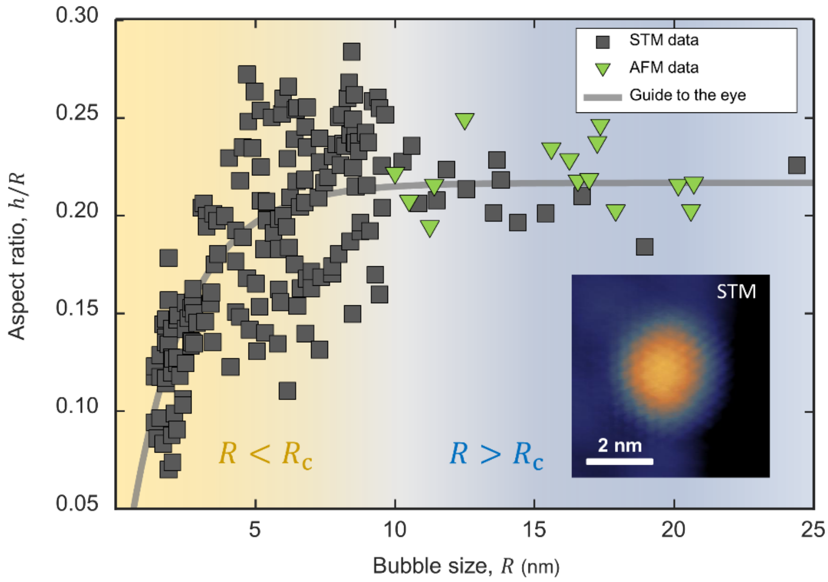
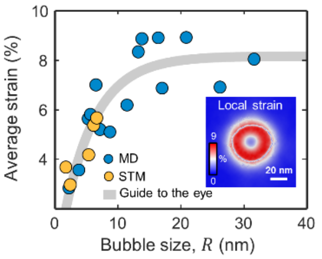
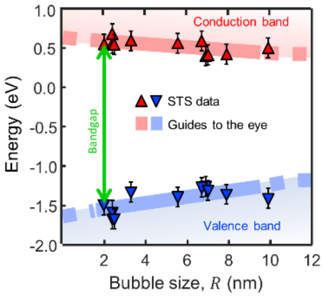
[3] A.A. Lyublinskaya, S.S. Babkin, and I.S. Burmistrov, *Phys. Rev. E* **101**, 033005 (2020)







C8

Integration of Ferroelectric and Freestanding 3D $SrTiO_3$ and 2D MoS_2 Nanomembranes for Multifunctional Devices

D. Sen[1], H. Ravichandran[1], M. Das[1], P. Venkatram[1], S. Choo[2], S. Varshney[2], Z. Zhang[1], Y. Sun[1], J. Shah[2], S. S. Radhakrishnan[1], A. Saha[1], S. Hazra[1], C. Chen[1], J. M. Redwing[1], K. M. Mkhoyan[2], V. Gopalan[1], Y. Yang[1], B. Jalan[2], and S. Das[1]*
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Ferroelectric field-effect transistors (FeFETs) have garnered considerable interest lately due to their impressive features, including non-volatile memory, low power consumption, and enhanced switching speed [1-2]. While progress has been made in developing energy-efficient FeFETs using ferroelectric materials like doped hafnium oxides [3], the post-deposition annealing process hinders integration at the back end. In this context, we capitalize on the benefits of van der Waals integration to develop reconfigurable FeFET based neuromorphic devices, functioning as both synapses and neurons. This is accomplished by integrating large-area freestanding STO nanomembranes and MOCVD grown monolayer MoS_2 films. We have achieved rapid polarization switching in under 20 ns at 100 K. Moreover, our electrical measurements projected >10 years of nonvolatile retention and endurance beyond 10^4 cycles. Additionally, we demonstrated 64 distinct memory states, in a single representative FeFET. Utilizing the temperature-dependent memory retention features, we introduced an adaptable device with the ability to shift from acting as an artificial synapse at lower temperatures to functioning as an artificial neuron at higher temperatures.

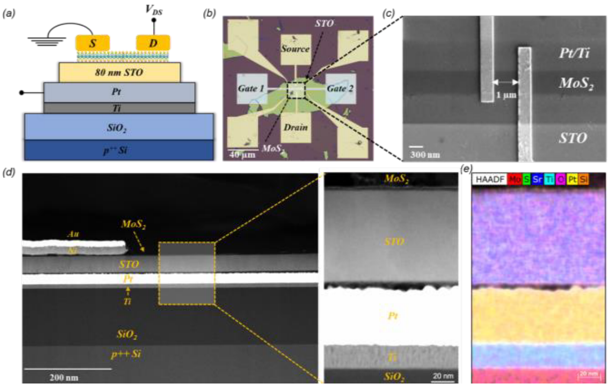

Fig. 1. (a) Device schematic, (b) top-view optical image, (c) scanning electron microscope (SEM) image of a representative FET based on 2D MoS_2/3D STO nanomembranes. (d) Cross-sectional STEM-HAADF image and (e) the accompanying EDS elemental mapping of the fabricated FET.

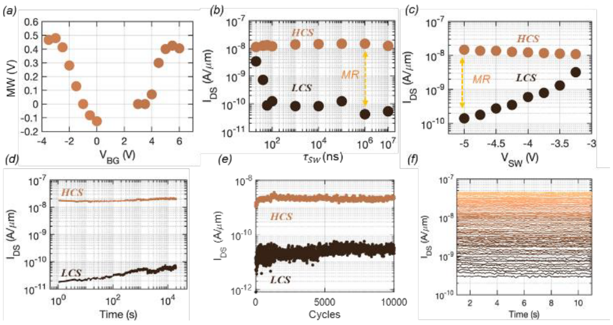

Fig. 2. (a) Memory window (MW) plotted as a function of the V_{BG}. (b) MW as a function of switching time (τ_{SW}). (c) MW as a function of V_{SW} for τ_{SW} = 20 ns. (d) Memory retention measured for 2×10^4 s. (e) Switching endurance for the STO film assessed for 10,000 cycles and (f) 64 memory states obtained by applying different amplitude of programming pulses of fixed τ_{SW} = 10 ms to form a 6-bit memory .

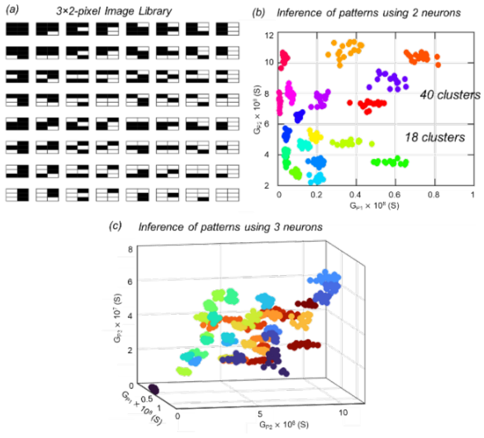

Fig. 3. (a) Image library consist of all possible patterns (2^6 = 64) corresponding to 3×2-pixel images. (b)-(c) Distribution of conductance values (G_p) for two and three neurons in classifying 64 patterns. Distinct clusters of 18 and 40 patterns emerge, underscoring the potential to discern an increasingly greater number of unique patterns by expanding the number of neurons.

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C9

Acousto-Optoelectric Spectroscopy on Transition Metal Dichalcogenides with Surface Acoustic Waves

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Surface acoustic waves (SAWs) have proven to be a multifaceted and efficient tool for the control of semiconductor nanostructures optical properties and the dynamical transport of charge carriers [1]. By integrating 2D semiconducting transition metal dichalcogenides (TMDCs) onto SAW-devices, we are able to investigate and control their interesting optoelectronic properties in a contact-free manner. SAW spectroscopy has already been used to probe the electrical transport inside CVD-grown MoS_2 on $LiNbO_3$ [2] and, in recent years, SAWs have been used to manipulate the emission of trions and excitons inside exfoliated TMDC monolayers [3,4,5].

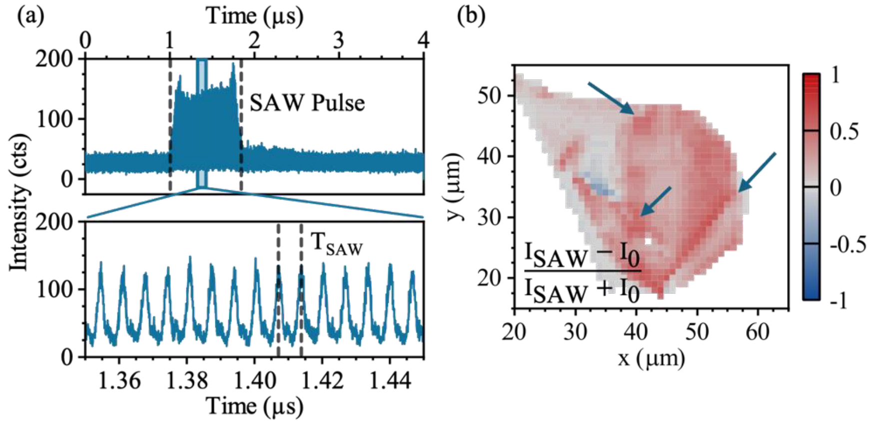

Figure 1 (a) Time-resolved measurement of the PL emission of the WSe_2 monolayer under a pulsed SAW modulation. Upper panel: The SAW is excited from 1µs to 1.8µs. Lower panel: SAW modulation of the photoluminescence emission of the WSe2 monolayer. (b) Mapping of the intensity ratio between the photoluminescence emission intensity during the SAW pulse I_{SAW} and before I_0.

To study the native interactions between a 2D semiconductor and the SAW, we integrated a WSe_2 monolayer flake onto a $LiNbO_3$ SAW device through a classical exfoliation process. After a measurement of the static emission of the monolayer, the impact of the SAW on its photoluminescence (PL) emission was systematically studied in the time domain. A clear enhancement of the PL intensity was observed (see Figure 1(a), upper panel). This enhancement is position-dependent and tends to be larger at the edges of the monolayer and close to defects (see Figure 1(b)). Most importantly, we observe a time-dependent modulation of the PL intensity clocked by the SAW's period (see Figure 1(a), lower panel). This finding provides unambiguous direct evidence of dynamic exciton modulation by the SAW. Moreover, the modulation of the PL emission during the SAW pulse exhibits distinct differences depending on the location within the monolayer, which are not reproduced in the static PL emission measured beforehand. This indicates that the SAW induced dynamics is much more sensitive to any type of localized change in the dielectric and strain environment. Our results show that SAW acouto-optoelectric spectroscopy can be a powerful tool to uncover the unavoidable inhomogeneities present in 2D TMDCs in experiments.

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C10

Infrared Magneto-Polaritonics And In-Situ Tuning of Exciton Dynamics In Two-Dimensional Crystals And Heterostructures In a Cryogenic Open Cavity

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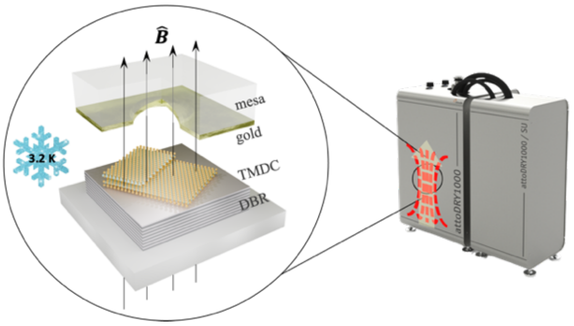
Optical resonators are a powerful platform to control the spontaneous emission dynamics of excitons and generate new quasi-particles of polaritons in solid-state nanostructures. In this talk, I will cover the recent advancement of our home-built low-temperature (3.2 K) open optical micro-cavity based on a liquid helium free cryostat that is also equipped with a superconducting magnet. New results of light-matter coupling of atomically thin semiconducting layers in both strong and weak coupling are summarized in the following:



(1). In the strong coupling regime, we study MoTe$_2$ monolayers and bilayers that are unique within the family of van-der-Waals materials since they pave the way towards atomically thin infrared light-matter quantum interfaces, reaching the telecommunication windows. We report emergent exciton-polaritons based on MoTe$_2$ monolayer as well as bilayer. Our experiments clearly evidence both, the enhanced oscillator strength and enhanced luminescence of MoTe$_2$ bilayers signified by a 38 % increase of the Rabi-splitting and a strongly enhanced relaxation of polaritons to low energy states. The latter is distinct from polaritons in MoTe$_2$ monolayers, which feature a bottleneck-like relaxation inhibition. The polaritonic spin-valley locking in monolayer as well as spin-layer locking in bilayer are revealed via the Zeeman effect, which we map and control via the light-matter composition of our polaritonic resonances.

(2). In the weak coupling regime, we study a MoSe$_2$-WSe$_2$ heterostructure that is integrated in the cryogenic open cavity to gain insights into fundamental optical properties of the emergent interlayer excitons. First, we utilize a low quality-factor planar open cavity and investigate the modification of the excitonic lifetime as on- and off-resonant conditions are met with consecutive longitudinal modes. Time-resolved photoluminescence measurements revealed a periodic tuning of the interlayer exciton lifetime by 220 ps, which allows us to extract a 0.5 ns free-space radiative lifetime and a quantum efficiency as high as 81.4 %. We subsequently engineer the local density of optical states by spatially confined and spectrally tunable Tamm-plasmon resonances. The dramatic redistribution of the local optical modes allows us to encounter a significant inhibition of the excitonic spontaneous emission rate by a factor of 3.2.

C11

Monolithic and heterogeneous three-dimensional (3D) integration of two-dimensional (2D) materials using dense vias

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The semiconductor industry is experiencing a tectonic shift with the adoption of three-dimensional (3D) integration, enabling the convergence of various technologies. Historically, through-silicon via (TSV) stacking has been the dominant approach to 3D integration, leading to the commercialization of 3D-stacked CMOS image sensors, 3D flash memories, and DRAM stacks. While TSV technology can achieve impressive interconnect (I/O) densities of up to 10,000 I/O per mm², further improvement requires the adoption of monolithic 3D integration (M3D). However, widespread use of non-silicon materials in M3D is pending. In this study, we showcase heterogeneous M3D integration using all-two-dimensional (all-2D) materials, achieving an interconnect density of 40,000 I/O per mm² with more than 500 devices in each tier. Additionally, our manufacturing process stays below 200°C, which is ideal for back-end-of-line (BEOL) integration. The M3D stack in our study includes graphene-based chemisensors in tier 2 and MoS_2 memtransistor-based programmable circuits in tier 1, tailored for near-sensor computing applications. A notable achievement in our work is the physical proximity between sensors and computing elements, which is less than 100 nm. This proximity far surpasses what is currently achievable with state-of-the-art packaging solutions.

Fig 1(a, b) shows cross-sectional images at different magnifications obtained using scanning transmission electron microscopy (STEM) in high-angle annular dark-field (HAADF) mode taken across the cross section of two consecutive 3D devices. In our M3D IC, tier 1 is composed of monolayer MoS_2 memtransistors, which serve as the primary computing components.

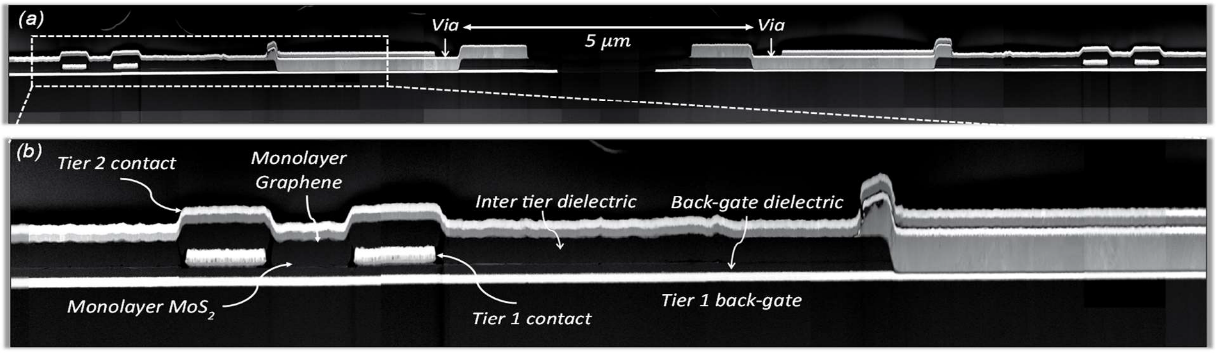

Fig. 1. (a) Stitched cross-sectional image and **(b)** a zoomed-in version obtained using scanning transmission electron microscopy (STEM) in high-angle annular dark-field (HAADF) mode taken at the cross section of two consecutive 3D devices.

C12

Exploring Light-Matter Interactions at the Interface of a 2D Antiferromagnetic Semiconductor Heterojunctions

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The growing interest in 2D magnetic semiconductors is driven by the vast possibilities for exploring new device concepts and for probing the unique optical and electronic properties of these materials and heterostructure interfaces. One field of particular interest is opto-spintronics, where spin-polarized carrier injection, transport or detection is driven or measured optically.

Here, we investigate the photoconductivity of devices comprising heterostructures of the antiferromagnetic materials family MPX_3, where M is magnetic cation Fe, Ni, Co or Mn, and X is a chalcogen S or Se. Particularly, the natural p-n heterojunctions along with their electronic optical characteristics provide a solid background to understanding the fascinating photoconductivity phenomena observed.

C13

Harnessing TBG for enantiomeric sensing of chiral molecules

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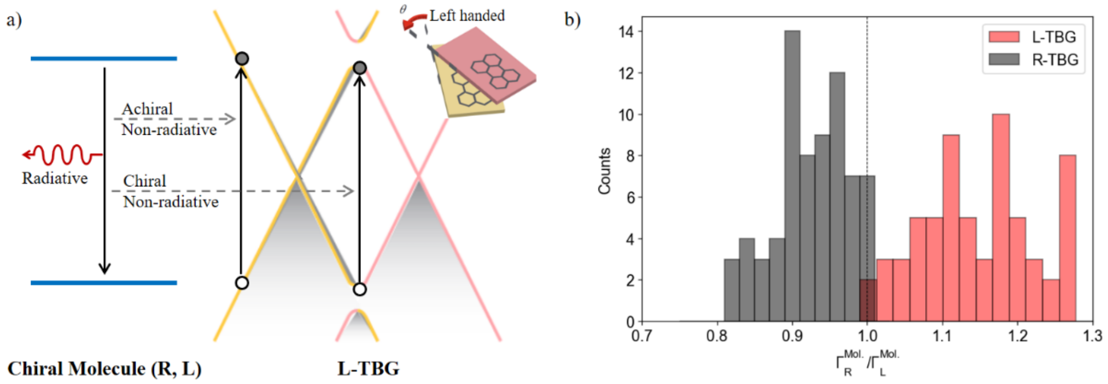
Selective sensing of chiral molecules is a key aspect in fields spanning biology, chemistry, and pharmacology. However, conventional optical methods, such as circular dichroism (CD), encounter limitations owing to weak chiral light-matter interactions [1]. Several strategies have been investigated to enhance CD or circularly polarised luminescence (CPL), including superchiral light [2], plasmonic nanoresonators [3] and dielectric nanostructures [4]. Nevertheless, a compromise between spatial uniformity and high sensitivity, without requiring specific molecular attachments, remains a challenge. In this work, we propose a novel approach using twisted bilayer graphene (TBG), a chiral 2D material with a strong CD peak whose energy is tunable through the twist angle [5-6]. As anticipated, energy transfer to TBG enhances the decay rate of the molecules [7]. By matching the CD resonance of TBG with the emission energy of the molecule, the decay enhancement depends on the electric-magnetic interaction, that is, on the chirality of both the molecules and TBG. Thus, the chirality of a molecule can be deduced from time-resolved photoluminescence measurements. This method demonstrates high sensitivity down to single layers of molecules, with the potential to achieve the ultimate goal of single-molecule chirality sensing, while preserving the spatial uniformity and integrability of 2D heterostructures.



a) Mechanism of energy transfer to TBG. The intervalley transition shows CD, thus resonant coupling is sensitive to the molecule and TBG chirality. Adapted from [5]. b) Decay rate ratio between the left and right handed enantiomers. The histogram is built from different spatial locations in the sample.

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C14

Circumventing the polariton bottleneck via dark excitons in 2D semiconductors

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The rich exciton landscape of transition metal dichalcogenides (TMDs) provides potential intervalley scattering pathways via momentum-indirect excitons [1]. These dark states have been extensively studied for bare TMD monolayers, where they can facilitate rapid energy relaxation, and have recently been demonstrated to play a key role in polariton absorption [2] and photoluminescence (PL) [3]. However, the relaxation dynamics for TMDs in the strong coupling regime is not as well understood. In particular, it is interesting to study the role of the polariton bottleneck effect, which impedes phonon-driven scattering into low-momentum states and can be detrimental for the development of room-temperature polaritonic devices and the investigation of polariton condensates. Using a microscopic Wannier-Hopfield approach [4], supported by detuning-dependent cryogenic PL measurements, we have explored the momentum- and time-resolved relaxation of exciton polaritons in an $MoSe_2$ monolayer integrated within a microcavity [5]. For a suitable cavity detuning, momentum-dark excitons provide an efficient reservoir to rapidly populate the polariton ground state via phonon-assisted scattering, and hence circumvent the bottleneck effect. Our detuning-dependent PL measurements confirm the existence of a polariton bottleneck at low temperatures and provide evidence for its circumvention by phonon-driven intervalley scattering from dark excitons as the cavity is blue detuned, in agreement with our theoretical predictions.

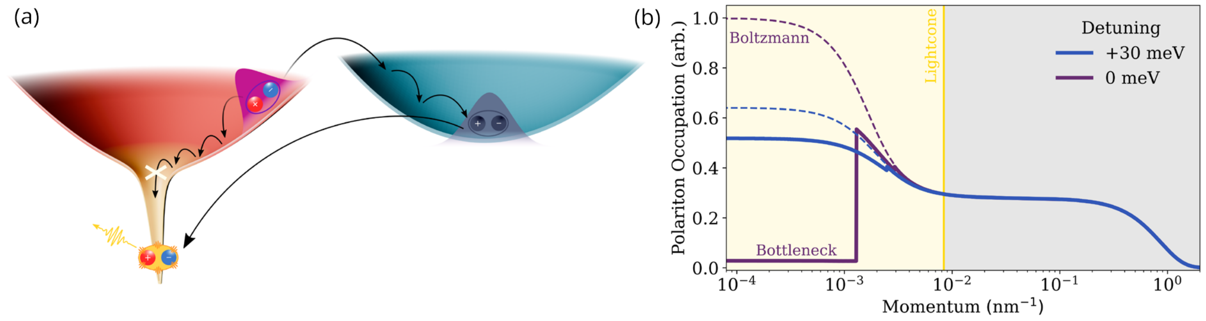

Fig 1. (a) Schematic of possible relaxation processes for the lower branch of a molybdenum-based exciton polariton. (b) Detuning dependence of the lower polariton occupation, revealing a bottleneck at low momenta for certain detuning values.

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C15

Quadrupolar Excitons in Natural MoSe$_2$ Bilayer

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Kenji Watanabe,[4] Alessandro Surrente,[1] Michał Baranowski,[1] Duncan K. Maude,[2]
Ermin Malic,[3] and Paulina Płochocka[1,2]

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2D Transition Metal Dichalcogenides (TMDs) emerged as a fascinatingly rich playground for studying excitonic physics, due to strong Coulomb interaction provided by the reduced dimensionality and a reduced dielectric screening in the monolayer limit. A further expansion to their vast potential is provided by multi-layer van der Waals homo- and hetero-structures, either natural or artificially stacked at an arbitrary twist angle. In recent years, the studies of homo- and hetero-structure based gated devices via the application of external electric field have proven especially fruitful. Recently, in addition to the commonly observed interlayer dipolar excitons (IX), another type of exciton species has been observed in TMD hetero-trilayers, namely the quadrupolar exciton, which is the result of the hybridization of two anti-aligned dipolar excitons [1].

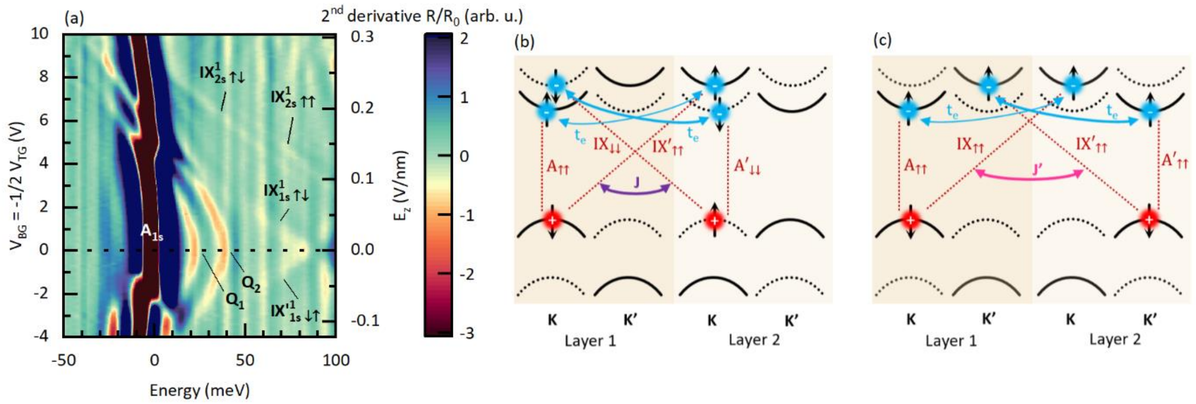

Figure 1 2H-stacked MoSe$_2$ bilayer. (a) Electric-field dependent 2nd derivative of reflectivity (R/R$_0$). (b) and (c) Schematics of coupling J hybridizing the opposite spin, same valley IXs, and J' hybridizing the IXs of the same spin and opposite valley, respectively.

Here, we investigated a simpler system consisting of a natural 2H-stacked MoSe$_2$ bilayer under electric field, in conjunction with theoretical modeling. In addition to the dipolar interlayer excitons, we observe clear signatures of two quadrupolar states (Q_1 and Q_2) as evidenced by their quadratic shift a electric field (Figure 1a), which is the first such observation in a homo-bilayer system. The Q_1 and Q_2 states originate from the hybridization of the anti-aligned spin-singlet interlayer dipolar states. To account for the formation and the splitting of the observed quadrupolar branches, an additional electron-hole exchange type coupling is included in our theoretical model. Two coupling mechanisms, labelled J and J', have been introduced to lift the four-fold degeneracy characteristic of homo-bilayers stemming from the valley and layer degrees of freedom. The unexpectedly large value of this coupling however, suggests existence of additional contributing effects, the nature of which requires further investigation.

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C16

Layer dependent magnetic ordering in two-dimensional magnetic insulator

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Abstract

Magnetic domain formation in two-dimensional materials offers insight into the fundamentals of magnetism and serve as a catalyst for the advancement of spintronics device technology. In order to propel these developments, its crucial to acquire understanding of the evolution of magnetic ordering at nanometer scale, as a function of number of atomic layers and applied magnetic field. In this study, we visualize few-layer annite ($KFe_3^{2+}AlSi_3O_{10}(OH)_2$) by employing a hybrid approach involving a scanning superconducting quantum interference device (SQUID) and an atomic force microscopy (AFM) probe. Annite is a naturally occurring van der Waals (vdW) magnetic insulators which incorporate local moment baring ions of iron (Fe) via in their octahedral sites. The simultaneous imaging capability of the SQUID-on-tip microscope, capturing both the surface features and its stray magnetic field, enabled us to establish correlations between layer thickness and magnetic ordering. External field dependent maps of annite's stray magnetic field reveal coercivity of 70 mT for the 2D flakes, and capture the domain formation and flipping in the external field.

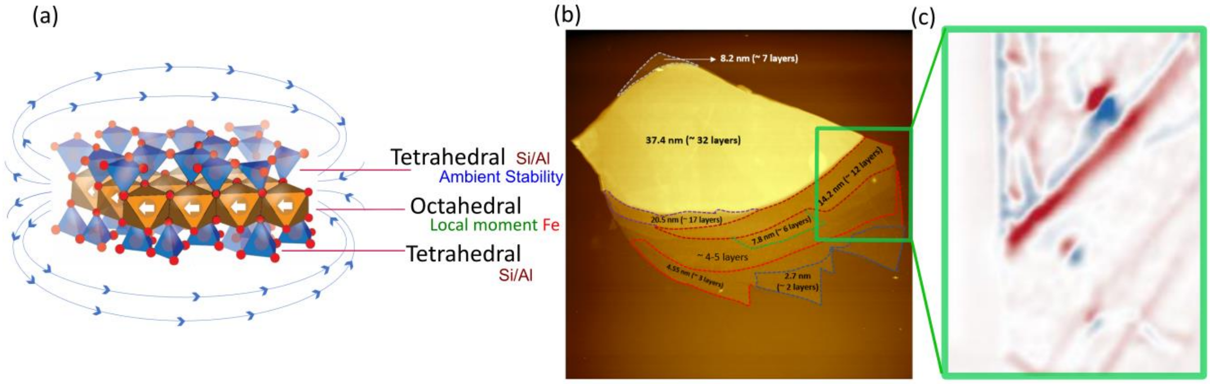

Figure: (a) Schematic diagram of monolayer annite showing in-plane magnetic field lines. (b) AFM scan of few-layer annite showing different layer thicknesses, (c) In-plane component of the stray magnetic field B_z measured above the sample in an applied in-plane field of -70mT.

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C17

Magnetic proximity interactions in the $CrCl_3$/hBN/WSe_2 heterostructures

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Monolayers (MLs) of WSe_2 are part of the semiconducting transition metal dichalcogenide (S-TMD) family, which low-temperature (T=5-10 K) photoluminescence (PL) spectra are composed of a series of excitonic lines, which have been widely investigated in the literature [1]. On the other hand, chromium chloride belonging to the family of magnetic layered materials is characterized by the ferromagnetic order with layers and the antiferromagnetic coupling between the layers with the in-plane spin alignment [2]. The combination of these two materials allows the study of the proximity effect [3].

In this work, we performed the photoluminescence (PL) experiment on the $CrCl_3$/hBN/WSe_2 heterostructure (HS), composed of a thick $CrCl_3$ layer, hBN spacer and WSe_2 ML. The spacer plays a crucial role in preventing charge transfer from WSe_2 to $CrCl_3$, as we presented in our previous work [3]. Measurements were performed at low temperature (T = 5 K), using 2.41 eV excitation energy in an out-of-plane magnetic field.

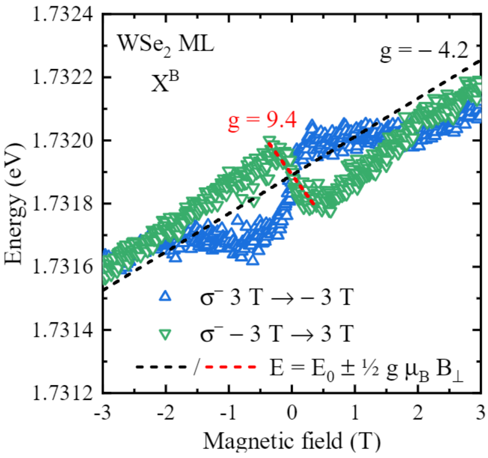

Figure 1: The magnetic field evolution of the neutral exciton (X^B) measured in the HS. The black line represents the Zeeman splitting function for the WSe_2 ML embedded in hBN flake based on the literature [1], while red dashed line is the fir using Zeeman splitting equation.

The Figure represents the energy dependence of the neutral exciton (X^B) measured on the HS in magnetic fields. Green and blue triangles denote the σ− polarization of the magnetic field course form 3 T to -3 T and from -3 T to 3 T, respectively. Within the range of small magnetic fields, an unusual behavior of the X^B transition is observed. The energy values exhibit non-linear dependence as a function of magnetic fields. Around |0.2| T, a sudden change in energy of approximately 3 μeV is observed. Using the standard equation for the Zeeman effect, describing the splitting into two circularly polarized components of the transition in the magnetic field [1], *i.e.* $E^{\sigma^{\pm}}(B) = E_0 \pm \frac{1}{2} g\mu_B B_\perp$, we found a g-factor of around 9.4 in this region. Furthermore, in magnetic field ranges of |0.2| T - |2| T and |2| T - |3| T, the data points form linear lines, each with different slopes. The magnetic field dependence of the X^B emission in the WSe_2 ML encapsulated in hBN flakes is characterized by the g-factor of around -4.2, which is represented by the dashed black line in the Figure. At the same time, the PL intensity of $CrCl_3$ shows a minimum at around |0.1| T. This is followed by the flattering of its intensity above |2| T, ascribed to a critical field [4], due to the change of the spin orientation in $CrCl_3$ from the intrinsic in-plane to along the applied out-of-plane magnetic field.

We propose that the departure from the linear dependence of the X^B energy in external magnetic fields can be understood in terms of the interaction between the magnetic $CrCl_3$ and the WSe_2 ML. It is conceivable that the unusual energy dependence at small magnetic fields is due to the presence of the $CrCl_3$ magnetization, while the increase in external magnetic fields causes the disappearance of the coupling between $CrCl_3$ and WSe_2. Finally, the change in the orientation of the spin alignments in $CrCl_3$ above the critical fields results in the standard Zeeman splitting of the X^B line. Our results emphasize the complexity of the magnetic coupling between magnetically ordered $CrCl_3$ and the WSe_2 ML due to the proximity effect, which understanding is key for future possible applications.

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C18

Inversion of magnetic anisotropy in thermally intercalated few-layer transition-metal thiophosphates: a magneto-optical investigation

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2D antiferromagnetic (AFM) materials of MPX_3 (M=first row transition metal, P=phosphorous, X=S, Se) family in pure and altered forms have attracted considerable attention in recent years, owing to their potential application in functional devices like spin filters, spin transistors, photodetectors, electrodes in solid state batteries and sensors [1,2]. While the extent of magnetic anisotropy and nearest-neighbor interactions control their effective magnetic properties [3], an alteration into the exchange interaction between adjacent magnetic centers by incorporating foreign entities can alter the ideal scenario [4], thus generating scope to control in plane and out of plane exchange interactions between the van der Waals layers. The present work aims at understanding the changes in interlayer and intralayer exchange interactions between antiferromagnetically ordered magnetic ions in layered materials via introduction of size compatible intercalates with electron-rich centers. Bulk and surface structural analyses using single crystal XRD, Raman. Electron diffraction techniques and XPS have delineated the effects of intercalation in the long-range and short-range structural arrangement of the material. Magnetic and electrical properties of pure and intercalated samples synthesized under different thermal conditions have been investigated to understand the orientation and effect of the intercalate (and its *in-situ* developed by-products) on the transport behavior of the lamellar systems. Magneto-optical measurements with temperature varying from 4K to 300K using a custom made confocal microscopic set-up have been performed to understand the correlation between magnetic and electronic properties of the 2D systems by virtue of different interfacial conditions of material layer-intercalate interaction. The understanding developed unveils the correlation between magnetic property with material-intercalate interaction, opening scope to tune spin dynamics of AFM materials for efficient quantum devices.

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C19

Exotic core-shell nanotubes synthesized via Van der Waals epitaxy

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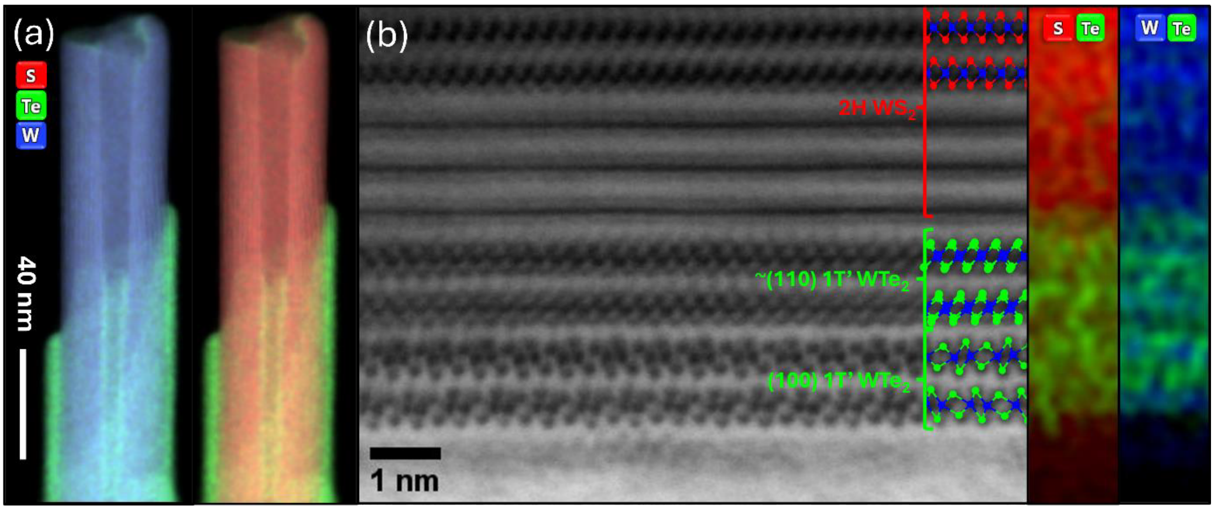
Van der Waals epitaxy[1] is a key synthetic strategy for obtaining various 2D heterostructures, including various transition metal dichalcogenides. Thanks to weak interactions between layers, possible lattice strain between divergent compounds is fully relaxed. In other words, heterolayers influence each other physically, mainly as layer alignment, orientations, or different interlayer distances.

In the series of experimental observations, the family of heterogeneous inorganic core-shell nanotubes based on Van der Waals epitaxial synthetic strategy was established. On the substrate, WS_2 multilayer nanotubes (2H phase) were deposited WTe_2, $MoTe_2$, ReS_2, and $ReSe_2$ layers (all usually found in 1Td or 1T' phases). In each of the formed WS_2@MX_2 core-shell nanotubes, a cascade of structures 2H-WS_2/ 1T'-MX_2 (or 2H) was observed by high-resolution electron microscopy analysis. In some cases, the so-called Van der Waals epitaxial cascade 2H-WS_2/2H-MX_2/1T'-MX_2 was found to be a stabilizing structural motif. The acquired materials promise modified (opto)electronic properties as well as topological effects.



High-resolution HRSTEM-HAADF/EDS micrograph of outer layers on WS_2@WTe_2 nanotube

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C20

Exploiting Point Defects in Two-dimensional Materials for Stochastic Encoding

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Defects significantly affect the reliability of electronic devices, especially as dimensions shrink in the microelectronics sector. Consequently, extensive efforts have been made to eliminate these defects from devices through the optimization of growth and fabrication processes. However, in the realm of emerging nanomaterials, such as two-dimensional (2D) semiconductors, a different scenario unfolds where point defects are considerably more prevalent than in silicon devices. The surface-only nature of 2D devices makes them particularly susceptible to detrimental effects due to these. In this study, we employ a multifaceted approach that encompasses atomistic imaging, density functional theory calculations, device modeling, and low-temperature transport experiments, to unveil the implications of point defects on random telegraph noise (RTN). Subsequently, using ab initio computational analysis and device-level modeling, we identify Se antisites (Se_W), shown in Fig.1a, and W vacancies (V_W) as plausible defect candidates to contribute to the observation of RTN in ultra-scaled WSe$_2$ field effect transistors (FETs) fabricated using metal-organic chemical vapor deposition (MOCVD) grown WSe$_2$ films. Both defects generate hole trapping states with charge transition levels (CTLs) close to the valence band edge. While most of the studies so far have focused on understanding the impact of point defects on device performance, it is worth noting that point defects have proven to be beneficial in numerous quantum and energy-harvesting applications. Surprisingly, their potential for computational purposes remains largely untapped. In our study, we harness defects in ultra-scaled 2D transistors as shown in Fig. 1b to accelerate an inference engine based on a stochastic spiking neural network, offering remarkable noise resilience. We utilized RTN shown in Fig. 1c to develop a stochastic encoder for image encoding. We demonstrate that medical MNIST (Modified National Institute of Standards and Technology) images shown in Fig. 1d, encoded into stochastic spike trains and fed into a pre-trained spiking neural network (SNN) shown in Fig. 1e, yield significantly higher inference accuracy (> 85%) compared to images with deterministic encoding (< 68%), especially when the images were inflicted with substantial noise as shown in Fig. 1f. In conclusion, our investigation underscores the critical importance of comprehending and leveraging intrinsic point defects in 2D materials as opportunities for neuromorphic computing.

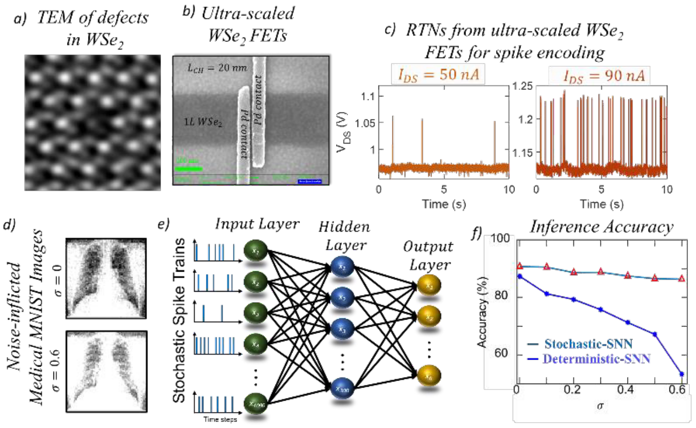

Figure 1. Stochastic encoder using defect dynamics in ultra-scaled WSe$_2$ FETs

C21

Distance Dependence of Mxene-Induced Fluorescence Energy Transfer and Applications in Single Molecule Biosensing

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This document provides instructions for preparing an abstract for “MIRSENS5” and is written in the format according to the guidelines given below.

MXenes, which were discovered in 2011, have become widely recognized as 2D materials that have potential applications in energy storage, electromagnetic shielding, and optoelectronics [1]. The energy transfer properties of these materials are still not fully understood, and this knowledge may have implications in various fields.

In this study, we utilized single-molecule fluorescence (confocal) microscopy and DNA origami nanopositioners to explore the distance-dependent intensity and lifetime of an emitter2 (ATTO 542) placed on transparent thin films made of spincoated $Ti_3C_2T_x$ MXene 2D flakes [3]. Each DNA origami structure was created to carry a single dye molecule at predetermined heights. We developed a specific immobilization chemistry for DNA origami nanostructures based on the interaction between glycine and MXene [4], which allowed us to control their orientation on the surface with precision.

Our research showed that when the dye was positioned between 1 nm and 8 nm from the surface, the fluorescence quenching followed a distance dependence of d^{-3}. These findings are consistent with the well-known Förster mechanism of near-field energy transfer with transparent conductors at the bulk level [5,6]. MXenes have the potential to serve as short-distance spectroscopic nanorulers for measuring biomolecular processes, providing a high level of sensitivity at a distance range that conventional energy transfer tools cannot reach. In this context, we demonstrate the utility of MXenes in single-molecule biosensing, focusing on model cell membranes as exemplary study systems. MXenes offer unique capabilities to uncover nanoscale dynamic processes intricately embedded within the ultrathin membrane architecture of cells.

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C22

Doping-control of excitons and magnetism in few-layer CrSBr

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In two-dimensional (2D) magnets, phenomena distinct from bulk magnetism have been revealed, such as sensitivity to charge doping and electric field in few-layer CrI_3 [1]. Within the class of 2D magnets, air-stable CrSBr stands out as an antiferromagnetic semiconductor with a high Néel temperature, excitons coupled to the magnetic order [2], and exciton-magnon coupling [3]. In this talk, I will present our work on doping-control of excitons and magnetism in few-layer CrSBr [4]. We demonstrate that both exciton and magnetic transitions are sensitive to field-effect charging, exhibiting bound exciton-charge complexes and doping-induced metamagnetic transitions. We further visualize magnetic domain formation induced by magnetic field or charge-doping at the metamagnetic transition all-optically by raster-scan reflectance imaging. Our work identifies few-layer CrSBr as a rich platform for exploring collaborative effects of charge, optical excitations, and magnetism.

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C23

High Energy Magnetic Excitons In CrSBr

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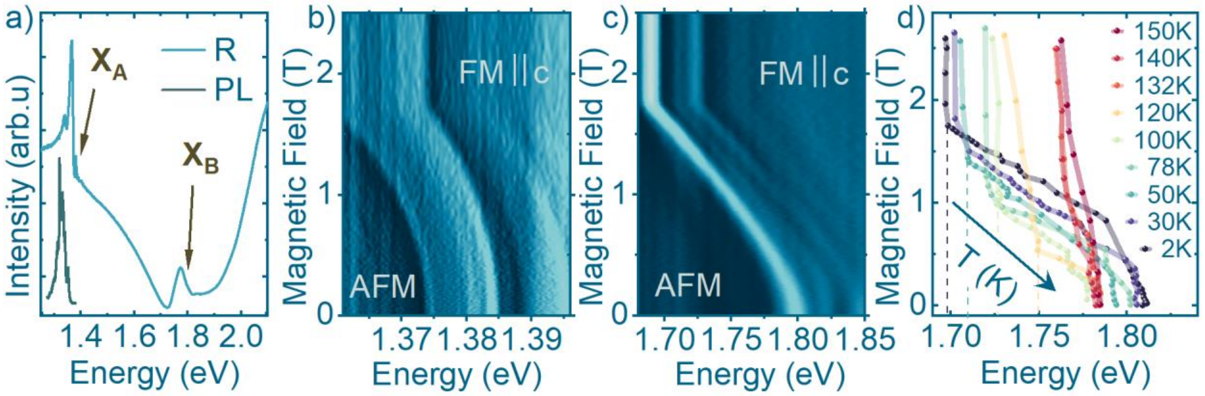
Chromium Sulfide Bromide (CrSBr) is a layered material that has recently gained significant interest due to its unique combination of magnetic and semiconducting properties and excellent chemical stability in ambient conditions.[1] In its pristine form CrSBr exhibits a layered structure with strong in-plane magnetic ordering below Néel temperature. Each layer couples antiferromagnetically to the neighboring layers. This antiferromagnetic state can be overcome using relatively low external magnetic fields (up to 2T) applied parallel to one of the three magnetization axes, affecting electronic structure significantly.[3]

This study focuses on the excitonic properties of CrSBr, under the influence of extreme magnetic fields, up to 85T parallel to the hard magnetization axis c. Firstly, we present results of the study in low field regime over a fundamental transition (X_A) as well as a higher excitonic species (X_B) coming presumably from a split valence band at Γ point in the Brillouin zone, both shown in photoluminescence (PL) and reflectivity (R) in 0T (fig.a). High energy exciton (X_B) is strongly coupled to magnetic order and shifts by significant 93 meV between the anti-ferromagnetic and ferromagnetic phase (fig.c). This is around the order of magnitude more than in the case of a X_A, which shift of 11 meV can be seen in false color plots of 1st derivative of R vs magnetic field (fig.b). This study is expanded by the investigation of these excitonic transitions in the FM phase, up to 85T, where high energy exciton experiences weak diamagnetic shift of $\sim 0.2 \mu eV/T^2$, in contrast to ground exciton state which shift in high magnetic field is not detectible. We ascribe this observation to different nature of two exciton states where the fundamental X_A is of Frenkel type while X_B is of Wannier type with its wave function expanding over neighbouring layers. Additionally, we investigate the temperature dependence of the excitons in high magnetic fields to understand how the competition between magnetic ordering and thermal disorder affects the excitonic properties of this material (fig.d).



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C24

Magnetic Properties of Non-van der Waals 2D Materials

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While 2D materials are traditionally derived from bulk layered crystals bonded by weak van der Waals (vdW) forces, the recent surprising experimental realization of non-vdW 2D compounds obtained from non-layered transition metal oxides [1] foreshadows a new direction in 2D systems research.

As outlined by our recent data-driven investigations [2, 3], these materials exhibit in particular unique magnetic properties owing to the magnetic cations at the surface of the sheets. Based on screening the AFLOW materials database first by a structural criterion for representatives similar to the experimentally realized systems and focusing then on magnetic compounds, we obtain 12 magnetic candidates (Fig. 1a). Despite of a few ferromagnetic systems, even for the antiferromagnetic representatives, the surface spin polarizations are diverse ranging from moderate to large values modulated in addition by ferromagnetic and antiferromagnetic in-plane coupling (Fig. 1b). At the same time, chemical tuning by surface passivation provides a valuable handle to further control the magnetic properties of these novel 2D compounds and eventually to even induce ferromagnetism as demonstrated by hydrogenation of 2D $CdTiO_3$ [4] (Fig. 1c). These features thus make these compounds an attractive platform for fundamental as well as applied nanoscience and in particular spintronics.

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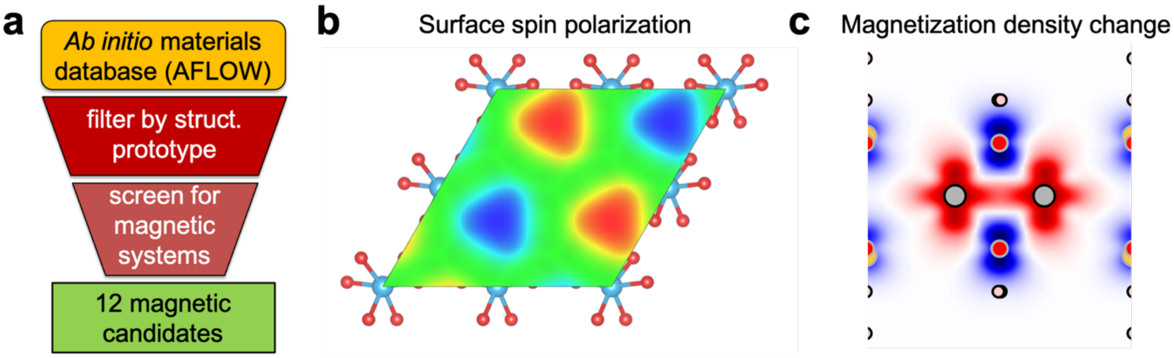

Figure 1. (**a**) Filtering for magnetic non-vdW 2D materials. (**b**) Surface spin polarization of $GeMnO_3$. (**c**) Magnetization density difference for $CdTiO_3$ due to hydrogenation indicating the onset of ferromagnetism.

C25

Understanding Domain Reconstruction of Twisted Bilayer and Heterobilayer Transition Metal Dichalcogenides through Machine Learned Interatomic Potentials

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In the study of twisted bilayer 2D materials, a detailed picture of the relaxations and layer-corrugations that occur due to interlayer interaction is crucial to predicting how their electronic and optical properties depend on twist angle and the resulting large-scale Moiré pattern [1]. As the relative twist angle between the layers approaches 0º, referred to as parallel (P) stacking, or 60º, referred to as antiparallel (AP) stacking, reconstructions occur to maximise the area of low-energy stacking domains, with a lattice of solitons of high-energy stacking connected by domain walls (DWs). We show that Machine Learned Interatomic Potentials (MLIPs) can provide the combination of accuracy and scaling required to obtain atomistic insight into this behaviour. In contrast to empirical potential methods, MLIPs based on higher-order equivariant message passing, as implemented in MACE [2], can provide very precise energetics of stacking, strain, shear and varying interlayer distances to exactly reproduce vdW-corrected DFT for systems dramatically larger than can be treated with ab initio methods. We predict, explain and quantify the domain reconstruction patterns for all like-chalcogen combinations of the Transition Metal Dichalcogenides MoS_2, $MoSe_2$, WS_2 and WSe_2 down to twist angles approaching 1º. We demonstrate effects including DW-bending in AP systems, and the "twirling" that occurs at the solitons in heterobilayers.

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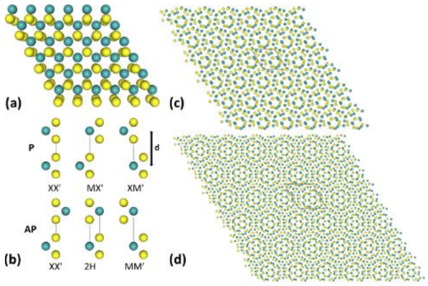

Figure 1. Schematics of the systems providing training data for the MLIP developed in this work (a) Monolayer MoS_2; (b) high-symmetry stacking configurations of bilayer TMDs, showing the three configurations in the P and AP cases; (c) the Moiré unit cell of the largest accessible twist angle (21.79º) and (d) the Moiré unit cell of the second-largest accessible twist angle (13.17º).

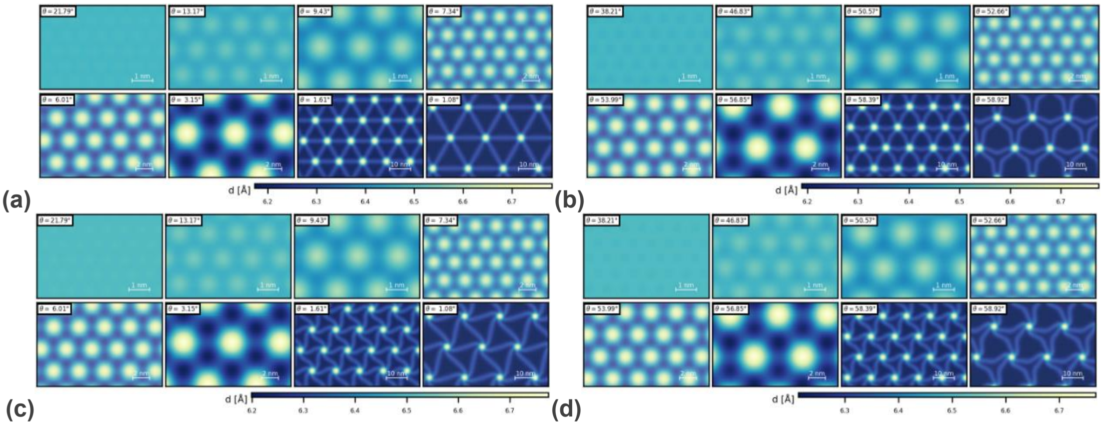

Figure 2. Interlayer distance maps for (a) P-MoS_2/MoS_2, (b) AP-MoS_2/MoS_2, (c) P-MoS_2/WS_2 and (d)AP-MoS_2/WS_2 at a range of twist angles.

C26

Giant Faraday Rotation in 2D Semiconductors

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Faraday rotation is a fundamental effect in the magneto-optical response of solids, liquids and gases. Materials with a large Verdet constant find applications in optical modulators, sensors and non-reciprocal devices.

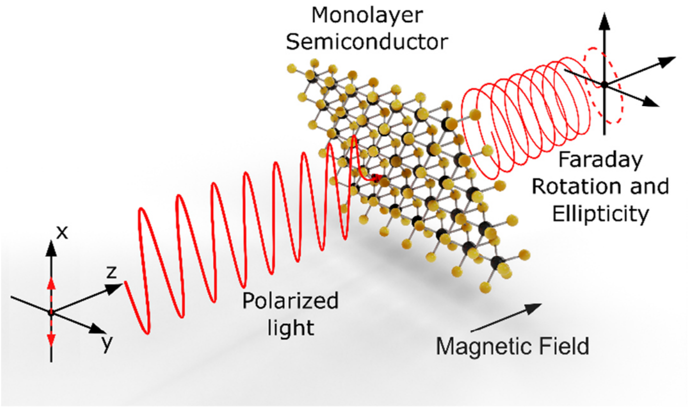

Figure 1. Schematic drawing depicting how linearly polarized light passes through an atomically thin semiconductor under a magnetic field and acquires Faraday rotation and ellipticity.

We measure Faraday rotation spectra around the neutral and charged exciton lines in hBN-encapsulated monolayers of WSe_2 and $MoSe_2$, and bilayers of MoS_2 under moderate magnetic fields ($B < 1.4$ T) [1] (see Fig. 1). For WSe_2 and $MoSe_2$ monolayers, the plane of polarization rotates by several degrees around exciton lines, resulting in a giant Verdet constant of $-1.9 \times 10^7 \mathrm{deg\,T^{-1}cm^{-1}}$ and $-2.3 \times 10^7 \mathrm{deg\,T^{-1}cm^{-1}}$, respectively. This is the largest measured Verdet constant in the visible/near-infrared regime. The giant Faraday rotation is due to the large oscillator strength and high g-factor of the excitons in monolayers. In comparison to monolayers, the Verdet constant reverses its sign for interlayer excitons in bilayer MoS_2 ($V_{\mathrm{IL}} \sim +2 \times 10^5 \mathrm{degT^{-1}cm^{-2}}$). We deduce the complete in-plane complex dielectric tensors of these materials, which is vital for the prediction of Kerr, Faraday and magneto-circular dichroism spectra of 2D heterostructures. For our measurements, we used a charge-coupled device-based Faraday rotation spectroscopy method for performing temperature-resolved spectroscopy on 2D materials on the microscale [2]. This method is about two-to-three orders of magnitude faster than state-of-the-art modulation magneto-spectroscopy methods, while providing a similar performance.

Finally, our results pose a crucial advance in the potential usage of two-dimensional materials in ultrathin optical polarization devices.

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C27

High-κ Wide-Gap Layered Dielectric for Two-Dimensional van der Waals Heterostructures

A. Söll[1§], E. Lopriore[2,3§], A. Ottesen[2,3], J. Luxa[1], G. Pasquale[2,3], J. Sturala[1], F. Hájek[4], V. Jarý[4], D. Sedmidubský[1], K. Mosina[1], I. Sokolović[5,6], S. Rasouli[6], T. Grasser[5], U. Diebold[6], A. Kis[2,3], and Z. Sofer[1]*

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The increasing demand for advanced electronic and photonic devices necessitates exploration into new dielectric materials compatible with two-dimensional (2D) heterostructures. Here, we present the synthesis, characterization, and application of a novel high-κ dielectric, LaOBr, for van der Waals (vdW) heterostructure devices. Employing a high-temperature flux growth method, we synthesized large, stoichiometric LaOBr crystals. These crystals were characterized by Raman, XRD, XPS, EDS, PLE, and subsequently exfoliated to yield flakes with a measured static out-of-plane dielectric constant of 9 and a wide bandgap of 5.3 eV.

Integration of LaOBr into vdW heterostructures as a gate dielectric revealed significant enhancements in device performance, including a high on–off ratio (Ion/Ioff > 10^{8}), minimal subthreshold slope (~85 mV dec^{-1}), and a low interface defect concentration (Dit ≃ 1.06 × 10^{12} cm^{-2} eV^{-1}). These features position LaOBr as a superior alternative to conventional high-κ materials such as Al$_2$O$_3$ and HfO$_2$, which are limited by interfacial challenges [1]. Moreover, we demonstrate that LaOBr can serve effectively as an encapsulating dielectric, for gated modulation of excitonic properties in devices based on monolayer transition metal dichalcogenides, showcasing its potential for future investigations of excitonic devices within high-κ dielectric environments. This research underscores the significant impact of LaOBr in advancing the functionality and integration of 2D materials, paving the way for next-generation electronic and optical devices.

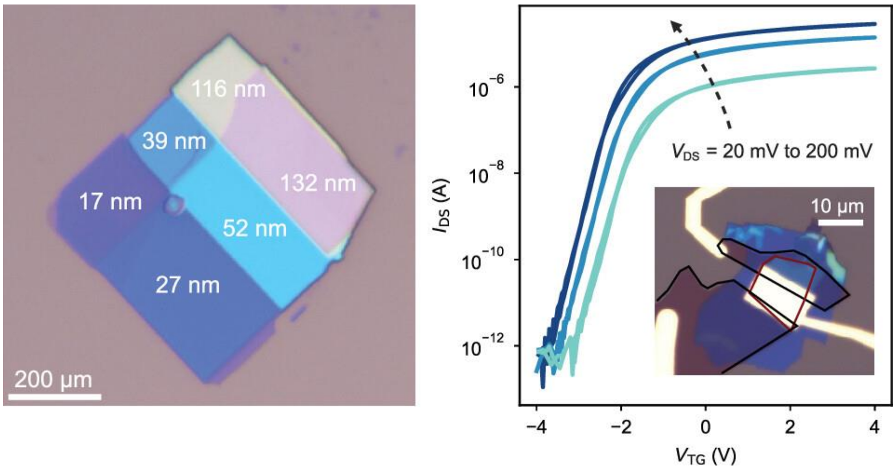

Figure 1. Exfoliated sheet of LaOBr; Transfer characteristics of MoS$_2$ transistor with LaOBr gate dielectric.

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C28

Metal-free magnetism in two-dimensional polymers

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Two-dimensional (2D) polymers with metal-free magnetism have garnered significant research interest due to their potential applications in organic spintronics. However, introducing stable spin-polarization and controlling magnetic interactions in these metal-free systems remains challenging due to strong electronic coupling and the closed-shell nature of most organic monomers. In this presentation, I'll present two approaches to introducing spin-polarization and regulating magnetic interactions in 2D polymers.

Firstly, chemical doping is used to introduce unpaired spins in narrow-band 2D covalent organic frameworks (COFs). [1] We demonstrate that forming a supramolecular charge-transfer complex is crucial for localizing electronic states and introducing stable paramagnetic centers into diamagnetic COFs. This approach reveals the anisotropic magnetic interactions within these 2D COFs and enables effective modulation of both spin-conduction and magnetic interactions with the spin centers.

The second approach involves utilizing stable radicals as building blocks, specifically triangulene—the smallest triplet-ground-state polybenzenoid with inherent spin-polarization. [2] By linking triangulene monomers into dimers and 2D polymers, we gain theoretical insights into controlling magnetic couplings and electronic structures. Enhanced magnetic couplings (J) of up to -198 meV have been achieved through rational design of chemical components in triangulene dimers. [3] Remarkably, ferromagnetic interactions are realized in nitrogen-centered triangulene dimers, beyond the predictive capability of Ovchinnikov's rule. Moreover, unique electronic structures, marked by a Dirac point flanked by twin flat bands, have been identified in triangulene-based 2D polymers. Manipulating the Fermi level could lead to metal-free ferromagnetism and a half-metallic characteristic. [4] These findings offer promising candidates for organic magnets and enhance our understanding of the complex interplay between electronic and magnetic states in metal-free systems.

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C29

Substitutional dopant engineering to achieve High-performance p-type Two-dimensional Field Effect Transistors

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The emergence of atomically thin 2D semiconductors like MoS_2 and WSe_2 marks a shift from traditional silicon-based CMOS technology [1,2]. While n-type FETs based on these materials meet IRDS standards, challenges persist for high-performance p-type FETs due to Fermi level pinning at metal/2D interfaces. Low work-function metals enhance n-type FETs but worsen contact resistance for p-type FETs. Transition metal selenides offer improved hole injection but reduce ON-state performance due to tunneling across the Schottky barrier. Innovative strategies are vital, particularly in degenerate doping beneath contacts, crucial for 2D FET design. Research shows pristine selenide flakes dominate n-type transport, while thicker doped flakes exhibit enhanced p-type doping with compromised gate control. Thinner flakes suffer from reduced doping effectiveness due to quantum confinement effects. Our novel FET architecture integrates thin channel layers with degenerately doped multilayer contacts, reshaping 2D FET engineering. This design achieves an impressive ON-current of approximately 85µA/µm, low R_C (~2 kΩ-µm), and an ON/OFF current ratio of 10^4. Integration of dual gate architecture and aggressive scaling further enhances performance, with an unprecedented ON-state current density of approximately 212µA/µm. This underscores the versatility and scalability of the proposed FET architecture for widespread adoption in advancing 2D FET technology.

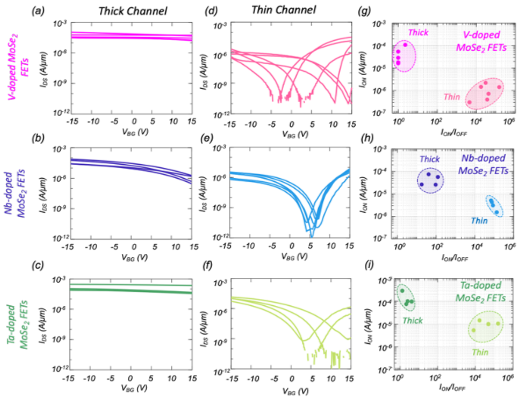

Fig. 1. Substitutionally doped p-type $MoSe_2$ FETs. Transfer characteristics of thin-channel **(a-c)** and thick –channel **(d-f)** V, Nb, Ta doped $MoSe_2$ FETs **(g-i)** I_{ON} vs. I_{ON}/I_{OFF} plots for V, Nb and Ta doped $MoSe_2$ FETs all channel thickness combined.

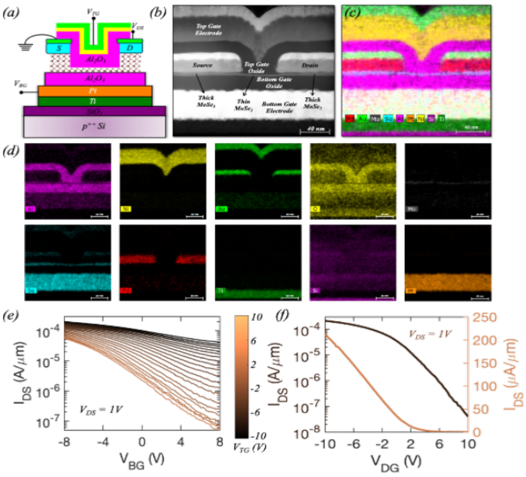

Fig. 3. High performance p-type dual-gated 2D FET (a) Schematic showing dual gated architecture on a scaled device which has been thinned down by oxygen plasma **(b)** cross-section HRTEM image of a dual gated device**(c)** corresponding EDX elemental mapping **(d)** elemental mapping of each element individually in the dual-gated structure. **(e)** Transfer characteristics obtained by sweeping V_{BG} from -8V to 8V while V_{TG} is varied from -10V to 10V. **(f)** Transfer characteristics when top and bottom gate are shorted (dual gate) and swept from -10V to 10V. Highest I_{on} achieved was 212 µA/ µm.

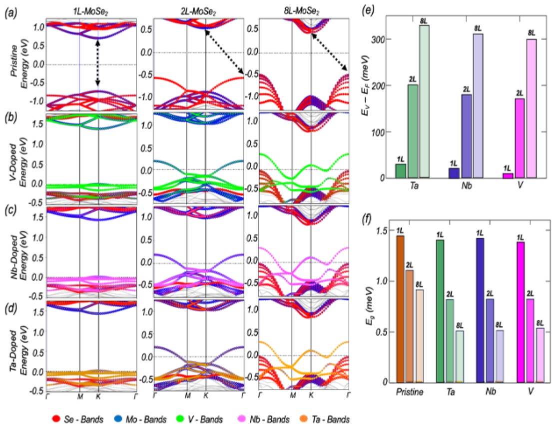

Fig. 2. Electronic band structure of pristine and doped $MoSe_2$. Energy band structure of single layer, double layer ad 8 layered **(a)** Pristine **(b)** V doped **(c)** Nb doped and **(d)** Ta doped $MoSe_2$. **(e)** Shows the separation of fermi level (E_F) from valance band maxima (E_V-E_F) for three layer-thicknesses (1L,2L,8L) with V, Nb and Ta **(f)** Band gap (E_F) for three layer-thicknesses (1L,2L,8L) with pristine and V, Nb and Ta dopants

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C30

Fabrication of high performance WSe_2 phototransistors and Si/MoS_2 pixel image sensors with High-Throughput Mechanical Exfoliation

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Van der Waals materials are a promising class of materials due to their layered structure, which allows easy exfoliation and isolation of atomically thin layers. This enables the fabrication of devices having thicknesses of a few nanometres. In our previous study, we invented a thin-film fabrication method: the high-throughput mechanical exfoliation. This is a scalable low-cost procedure to provide large-area films made from nanosheets of van der Waals materials having remarkable electronic and optical properties[1]. In the present work, we have focused on the integration of the high-throughput mechanical exfoliation into two different applications. First, we demonstrated the large-scale fabrication of high-performance phototransistors made from thin films of WSe_2, and second, we presented the fabrication of Si/MoS_2 based pixel image sensors. WSe_2 phototransistors feature a fast response time of less than 1 ms and a high photoresponsivity of up to 34 A/W. While as-fabricated WSe_2 transistors exhibit ambipolar characteristics with similar electron and hole conduction levels, high vacuum annealing suppress the hole conduction and causes a significant enhancement of the electron conduction current. Our measurements show that the fabricated transistors exhibit mobilities up to 3 cm^2 V^{-1} s^{-1} with a 10^4 on/off ratio. In the second part of the study, we presented the fabrication of the compact pixel image sensor consisting of the array of Si/MoS_2 based photodiodes. The heterojunction formation was achieved by the deposition of high-throughput mechanically exfoliated MoS_2 films on a silicon platform formed by etching the oxide layer of silicon substrate with the photolithograpy technique. We then investigated the sensing capabilities of the fabricated sensors to generate digital images. Overall, in this study we demonstrate the capability of the high-throughput mechanical exfoliation technique for applications in different fields.

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C31

Linearly-polarized electroluminescence in van der Waals heterostructures

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Germanium sulfide (GeS) is an anisotropic layered material with a direct band gap around 1.78 eV [1]. GeS possesses a low-symmetry orthorhombic crystal structure analogous to that of black phosphorous. The optical response of GeS was systematically investigated using experimental techniques, such as photoluminescence, reflectance contrast, and Raman scattering [2]. Electroluminescence (EL) studies have not been reported in the literature yet. The investigation of EL anisotropy is an innovative aspect of this study.

Here, we investigate the EL response of GeS assembled in two types of structures: with tunnel barriers and without tunnel barriers. Thin layers of hexagonal BN (hBN) act as tunnel barriers. The bias voltage was applied to the graphene flakes via metallic contacts. The photos of the samples and the structures schemes are in Figures a) and b).

The EL of the sample with tunnel barriers is apparent at 1.77 eV, which is associated with the neutral excitonic transition in GeS, see Figure c). It is intriguing that the structure without tunnel barriers does not have EL from the neutral exciton. However, there are observed emissions at higher energies at 2.04 eV and 2.30 eV (see Figure d)), which coincide with higher energy transitions around the Γ point. In the sample with barriers, GeS exhibits linearly polarized EL along the armchair crystallographic direction, which is in agreement the corresponding photoluminescence response [2].

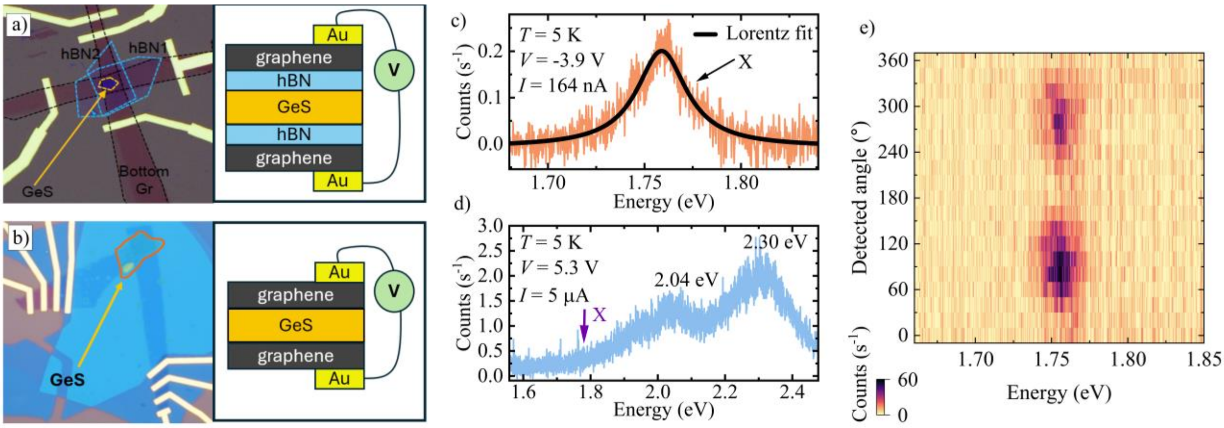

Figure: The optical images and schemes of the samples a) with tunnel barriers and b) without tunnel barriers. EL spectra measured on sample c) with tunnel barriers and d) without tunnel barriers. e) The false color map of the polarization-resolved EL from the sample with tunnel barriers.

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Freestanding Ferroelectric Perovskite Oxides: from High-performance Transistors to Tunable Exciton Emission

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Research interest in freestanding complex oxides has grown rapidly recently. Extending the possibilities of classic 2D materials by adding freestanding 3D layered materials is of great interest for (opto-)electronics. These oxides are offering advanced functionalities unthinkable for standard 2D oxides, such as hBN. Combining these materials with 2D semiconductors gives rise to rich new physics and improved electronic device systems. [1] Specifically, the high-k ferroelectric perovskite $BaTiO_3$ has drawn attention as a novel freestanding material for transistors and novel memory architectures. [2] By leveraging the unique properties of this material, we aim to develop advanced electronic structures with enhanced performance and functionality.

After growth of BTO and its delamination we can easily transfer the freestanding material of desired thickness to any substrate. By combining it with MoS_2, a two-dimensional direct-bandgap semiconductor, we enhance the optoelectronic properties of MoS_2. Assembling the structure into a field-effect transistor results in large on/off ratios, high field-effect mobility and high subthreshold-slopes (Figure 1). Furthermore, this structure can be used as a ferroelectric field-effect transistor in the field of non-volatile memory devices, due to the ferroelectric nature of BTO. [3] Utilizing the same combination of materials in a different device structure, we are able to largely control excitonic behavior of the monolayer MoS_2 by electrostatic gating through BTO. Photoluminescence measurements at room temperature reveal highly tunable light emission between the A exciton and its trion, as well as tunable trion binding energy over a small range of gate voltage with considerably lower power consumption compared to the same structure with hBN dielectric (Figure 2).

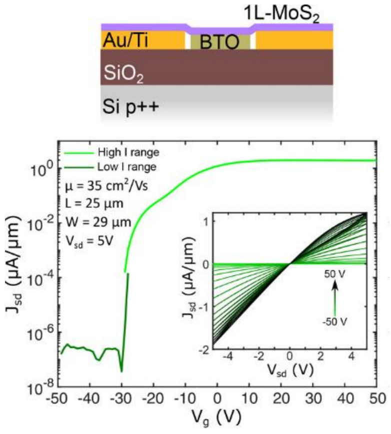

Figure 1: High-performance MoS2/BTO transistors. [3]

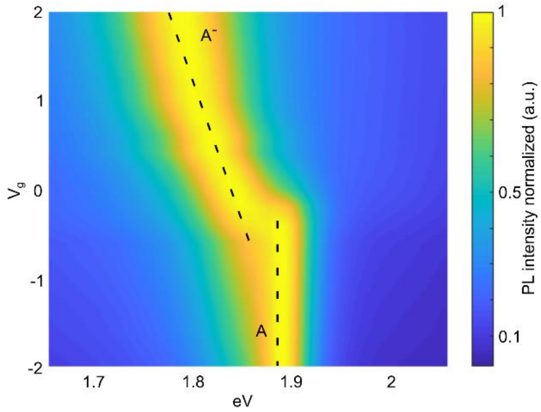

Figure 2: Tunable excitonic emission of MoS2 via BTO gating at room temperature.

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Nanotubes and Other Nanostructures of VS_2, WS_2, and MoS_2: Structural Effects on the Hydrogen Evolution Reaction

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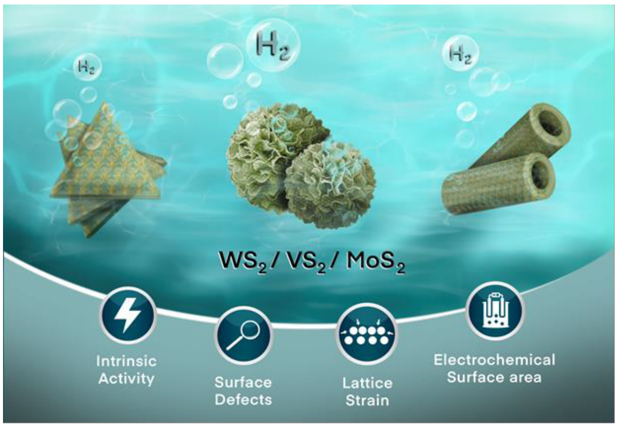
Vanadium sulfide (VS_2) is a layered transition metal dichalcogenide (TMD), comparable in crystal structure to the well-known MoS_2 and WS_2. Theoretical predictions attribute much potential to VS_2, since it is metallic-like and has an active basal plane, essential for catalytic performance. However, it is much less studied than other members of the TMD family due to the difficulties in synthesizing specific structures with controlled properties. Here we present unique structures of VS_2 nanotubes and conduct a comparative study with other well-known inorganic nanotubes and nanostructures of MoS_2 and WS_2. We evaluate the effect of the curvature and strain, the abundance of surface defects, and the availability of surface sites in various structures by electrochemical methods. We show that MoS_2 has the best intrinsic activity, which is enhanced by an extensive electrochemical surface area. The woven-like structure of the MoS_2 nanotube walls provides a combined effect of strain, crystallinity, and defects. For WS_2 structures, the strained surface of the nanotubes results in sites with higher intrinsic activity than the edge sites, but structures such as the nano-triangles, which provide a higher number of edge sites, exhibit competing activity. As for the VS_2 structures, although theoretical calculations predict optimal active sites for the hydrogen evolution reaction (HER), they are extremely sensitive to stoichiometry variations that hamper their catalytic activity. Our findings contribute insights to the improvement and design of VS_2–based nanocatalysts for the HER and shed light on the general factors that govern the activity in the unique TMD nanotubes family.



C34

Engineering Functionalized Mxene-based Interfaces for Superior Photocatalytic Hydrogen Evolution

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In the ongoing quest for sustainable energy solutions, photo- and electrocatalytic hydrogen production using novel materials is emerging as a promising green technology. This approach leverages various 2D materials, from classic graphene to transition metal dichalcogenides (TMDCs) and even novel discoveries like germanene and MXenes. Recent research has shown that combining these 2D materials into heterostructures unlocks even more intriguing properties, making them ideal for solar-driven water splitting. This study investigates a specific heterostructure made of MXene-TMDC nanostructures [1]. Electrodes loaded with this composite achieved impressive results, exhibiting low energy requirements for both hydrogen and oxygen evolution at high current densities, all while maintaining stability for over 100 hours. The MXene-based heterostructure displayed impressive performance in both hydrogen evolution (HER) and oxygen evolution (OER) reactions. Notably, illumination under 420 nm LED light, it achieved a photocurrent density of 120 µA/cm². As a water-splitting photocatalyst, it exhibited a significantly lower overpotential, reaching around 87 mV for HER and 430 mV for OER at 100 mA/cm², signifying the ability of material to drive water splitting with enhanced efficiency and effectiveness.

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Flatlands

Poster presentations

P1

Electrical characteristics of field-effect transistors based on MoSSe alloys

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Two-dimensional (2D) semiconductor materials, particularly transition metal dichalcogenides (TMDs) and their alloys, have recently attracted considerable scientific and technological interest due to their unique optical and electrical properties, which are dependent on the thickness of the structure. This allows them to find a wide range of applications in optoelectronics and sensors, among others. In the present study, the electrical properties of ultrathin field effect transistors (FET) based on $Mo(S_XSe_{1-X})_2$ crystals were investigated. The samples were prepared using mechanical exfoliation and the dry transfer method [1,2]. To characterize the number of layers, Raman spectroscopy measurements were performed, which prove that single crystal layers were obtained. Specially prepared SiO_2/Si substrates with 5 µm separated gold planar electrical contacts were used to fabricate the structures. The electrical properties of devices, including 2D semiconductors, depend nonlinearly on temperature (fig. 1). The FET has the best performance at $T = 350$ K, for which the highest drain current (I_D) and on/off current ratio (1.3×10^5) were obtained. The lowest on/off current ratio is 1.4×10^3 at $T = 450$ K. For comparison, this parameter for MoS_2 at room temperature is 1×10^6 [3]. In addition, the temperature significantly influences the threshold voltage (V_T), which varies nonlinearly from -5.5 V for $T = 400$ K to 5.0 V for $T = 300$ K.

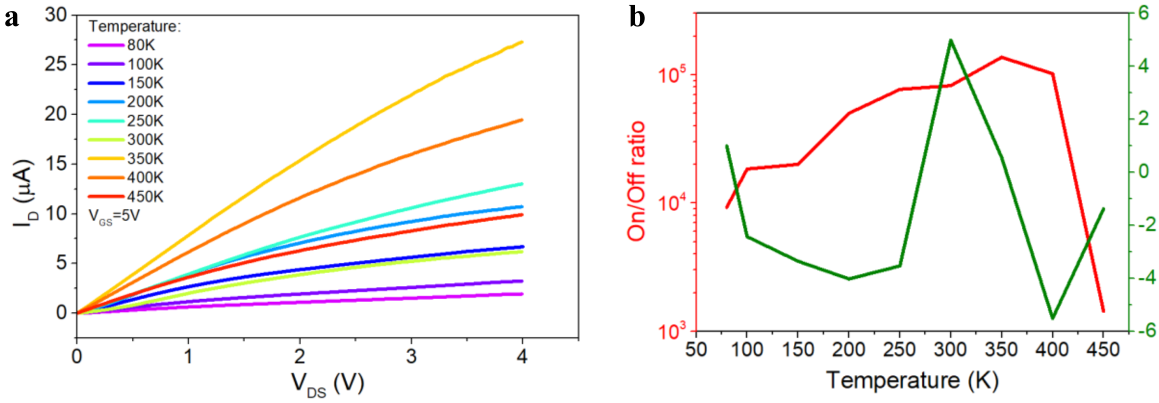

Fig. 1: Effect of temperature on the properties of single-layer $MoS_{0.82}Se_{1.18}$ FET: (**a**) output characteristics at constant gate-source voltage, (**b**) threshold voltage (V_T) and on/off current ratio.

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P2

Structural Dependence of Nitrogen Reduction Reaction (NRR) Activity on Mo_2TiC_2 MXenes

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Electrochemical reduction of nitrogen (N_2), as an environmentally friendly alternative for producing ammonia (NH_3), not only permits the use of the readily available water as a source for protons under mild conditions, but also contributes significantly to driving the commercialization of renewable energy technologies, thereby, bridging the gap between peak power production and peak energy demand [1-3]. However, the identification of non-precious metals and high-efficiency electrocatalysts remains the major challenge towards commercialization of such energy technologies. Amongst the extensively explored family of two-dimensional (2D) materials, MXenes have been found to demonstrate great potential as electrocatalysts for NRR [4-6]. In this work, the dependence of the NRR process on molybdenum-based MXenes ($Mo_2TiC_2T_x$) with different termination surfaces (T_x: -OH, -F) was investigated via the measurement of activity, operational durability, and selectivity to hydrogen evolution reaction (HER). In alkaline media, the results revealed that -OH termination plays a valuable role in tuning the NRR chemistry through provision of hydrogen (H) atoms to the intermediates, thus further participating in NRR process. As a result, the OH-terminated Mo_2TiC_2 exhibited NH_3 yield rate of 30.1 $\mu g.h^{-1}.mg_{cat}^{-1}$ with Faradaic Efficiency (FE) of 18.34 % at -0.62 V (vs RHE), good hinderance to parasitic HER, and good durability over an 8 h operation period. On the contrary, the F-terminated Mo_2TiC_2 displayed low NH_3 yield rate of 12.6 $\mu g.h^{-1}.mg_{cat}^{-1}$ (FE≈9.75%) and poor selectivity between NRR and HER processes. In addition to providing new insights into the deployment of active 2D materials in advanced sustainable NH_3 production, the study also elucidates the crucial role of surface functionalization of MXenes in evaluating NRR performance.

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P3

Scanning Electrochemical Microscopy on Graphene Oxide Bombarded by Metallic Ions

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Energetic ion beams offer an intriguing approach to modifying the structure and properties of various 2D materials. Graphene oxide, owing to the presence of diverse functional groups, emerges as a promising candidate for such investigations. In this study, we explored the interaction of graphene oxide, prepared via graphite oxidation, with energetic ions. Carbon ion beams with an energy of 20 keV and an ion fluence of 10^16 and 10^12 ions cm^-2 were utilized to bombard the surface of graphene oxide foil, aiming to alter its surface composition and structure. A range of analytical techniques, including scanning electron microscopy, Raman spectroscopy, atomic force microscopy, and photoelectron spectroscopy, were employed to demonstrate that such treatment leads to an overall reduction of the oxygen functional groups. Furthermore, it was observed that higher ion fluences result in a greater degree of reduction. Subsequently, the reduced samples were probed using scanning electrochemical microscopy in conjunction with two electrochemical probes – $K_4[Fe(CN)_6]$ and $[Ru(NH_3)_6]Cl_3$. The results clearly illustrate that $[Ru(NH_3)_6]Cl_3$ is significantly more sensitive to surface composition changes, providing clear contrast between bombarded and unbombarded areas. In conclusion, our study highlights the efficacy of energetic ion bombardment in reducing oxygen functional groups in graphene oxide, with higher ion fluences leading to greater reduction, and underscores the sensitivity of $[Ru(NH_3)_6]Cl_3$ as an electrochemical probe for detecting surface composition changes in such modified materials.

P4

Optical Transitions of Some MPS_3 Layered Compounds Under Hydrostatic Pressure

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Following the great success of transition metal dichalcogenides (TMDs), transition metal thiophosphates (TMTs) with formula MPS_3 have attracted considerable attention due to their outstanding electronic, structural, and magnetic properties. The wide spectrum of optical absorption, ranging from near infrared to ultraviolet [1], has sparked interest in utilizing MPS_3 materials for photodetectors and optoelectronic devices. Due to the weak van der Waals forces between the layers of such crystals, they can be very susceptible to external stimuli such as pressure, temperature, and magnetic field. For this reason, we combine the applications of hydrostatic pressure with absorption spectroscopy and investigate the optical transitions of some MPS_3 compounds for which M = Mn, Fe, Co and Ni. Apart from the same crystal structure and space group (monoclinic C2/m), all of them possess incomplete 3d orbitals, with occupation number varying from 5 to 8 from Mn to Ni, leading to optical transitions below the absorption edge, the so-called d-d transitions, which can be explained by crystal field theory. It has been observed that the absorption edges move towards lower energies with increasing pressure, while the d-d transitions shift to higher energies (except in the case of $MnPS_3$, in which both transitions redshift). Finally, we combine our experimental data with density functional theory calculations to assign the observed transitions to the corresponding points of the Brillouin Zone.

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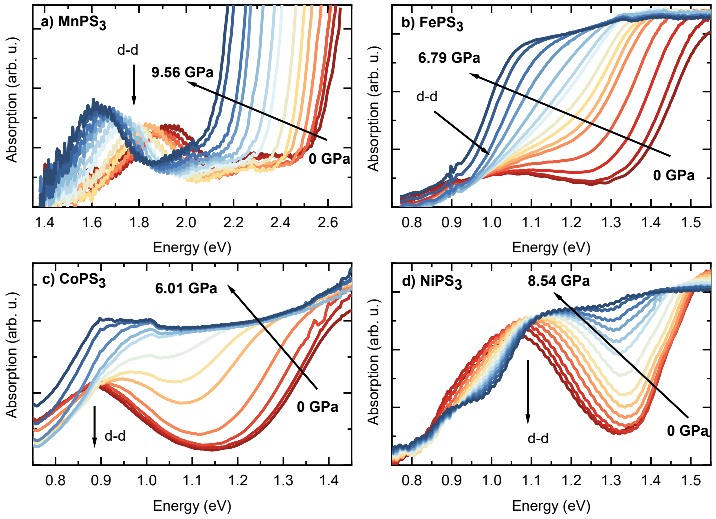

Fig. 1: Absorption spectra of a) $MnPS_3$, b) $FePS_3$, c) $CoPS_3$ and d) $NiPS_3$ at room temperature with pressure dependence.

P5

Resonant exciton scattering reveals Raman forbidden phonon modes in layered GeS

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The IV–VI layer compound like germanium monosulfide (GeS) with an anisotropic puckered crystalline structure has recently attracted much attention due to its unique optical and electronic properties [1]; however, exciton–phonon interactions were only superficially elucidated.

Here, we study the resonant Raman scattering and the photoluminescence of the optically active Γ-exciton in layered GeS flakes and evaluate the exciton and phonon responses on variations in the excitation energy, laser-light and emission polarizations, temperature, and laser power. A double-resonance mechanism allows for observing Raman forbidden (dark) first- and second-order longitudinal-optical phonon modes [2]. The symmetries and energies transitions are moreover calculated by Quantum ESPRESSO software suite [3] using density functional theory (DFT) in plane wave approximation for electronic structure and density functional perturbation theory (DFPT) for phonon calculations. For (quasi)-resonant exciton excitation, the selection rules become relaxed so that a fourth-order Fröhlich intraband process is mediated by the scattering of the electron with a longitudinal-optical and an acoustic phonon. Our results demonstrate considerable coupling between phonons and photogenerated carriers in GeS flakes and the high efficiency of multiorder scattering in optical processes.

[1] C. H. Ho, J. X. Li, *Adv. Optical Mater* **5**, 1600814 (2017).
[2] J. Jadczak, J. Andrzejewski, J. Debus, C. H. Ho, L. Bryja, *The Journal of Physical Chemistry Letters* **14** (17), 3986-3994 (2023).
[3] I. Carnimeo, F. Affinito, S. Baroni, O. Baseggio, L. Bellentani, R. Bertossa, P. D. Delugas, F. Ferrari Ruffino, S. Orlandini, F. Spiga, P. Giannozzi, *Journal of Chemical Theory and Computation* ***19****(20), 6992-7006 (2023).*

P6

Optical Transmission and Photomodulated Spectra Analysis of VdWs crystals placed on Fiber Tips

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Optical transmission is a key method for material characterization, allowing for simple determination of absorption spectra. Moreover, by introducing a modulated laser beam that evokes a perturbation in the material, photomodulated transmission spectra can be measured, which also enables the observation of optical transitions[1]. Thinning vdWs crystals, such as MoS_2, is often necessary to allow light transmission through higher-energy portions of the absorption spectrum, thereby revealing optical transitions A and B beyond the indirect absorption edge. However, this approach can be challenging. Optical fibers, through light confinement, offer here a solution by creating micro-laboratories that enable precise absorption measurements, even down to monolayers. In our study, we obtained the methodology of transferring TMDC materials on fiber tip and explored absorption properties of thin samples by observing excitons A and B. We also employed a backlight laser beam, which caused changes in absorption spectra through controlled heating, thereby providing insights into the effect of temperature variations within the sample. Furthermore, photomodulated transmission (PT) measurements using the lock-in technique were also conducted to observe the mentioned effects directly. The results of PT experiments were compared with absorption changes obtained through spectrometer analysis.

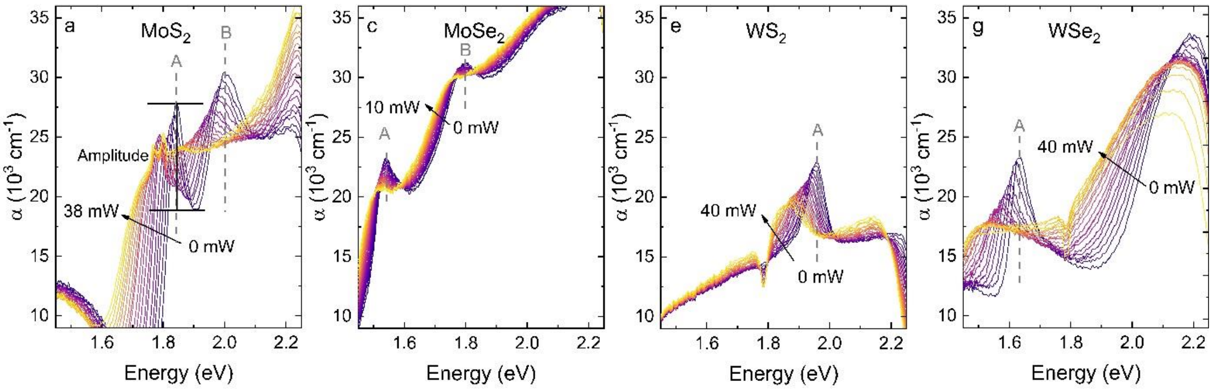

Fig. 1 Absorption spectra with changing laser power of backlight beam measured for MoS_2 (a), $MoSe_2$ (b), WS_2 (c), and WSe_2 (d).

[1] Kudrawiec, R. & Walukiewicz, W. Electromodulation spectroscopy of highly mismatched alloys. *Journal of Applied Physics* **126**, 141102 (2019).

P7

Strain Engineering of $MoSe_2$ Monolayers on GaAs Nanomembranes

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Transition metal dichalcogenides (TMDs) possess an excellent mechanical robustness and flexibility, which enable them to withstand strains as high as 10% before reaching the fracture point. Therefore, strain engineering has become a particularly attractive tool to tailor their electronic and vibrational properties or to preferentially funnel photoexcited carriers towards defects, which act as single photon emitters [1]. One of the approaches to site-control these quantum light emitters is the deposition of TMD monolayers on patterned substrates [1], thereby imposing spatially controlled strain on the two-dimensional layers.

So far, patterned substrates consist mainly of SiO2 nanostructures, which, however, suffer from surface charge instability. This provokes spectral wandering and blinking of single photon emitters. Here, we explore an alternative approach to deterministically imposing strain on TMD layers by making use of high-quality, epitaxially grown III-V semiconductor nanostructures.

We show a successful deposition of $MoSe_2$ monolayer on 100 nm high GaAs nanomembranes with 10 μm pitch in Fig. 1a. By performing photoluminescence (PL) spectroscopy and PL mapping, we show that the TMD monolayer deposited on GaAs nanomembranes was effectively strained. This is demonstrated by the observed redshift of the exciton PL peak, as shown in the false color PL map of Fig. 1b.

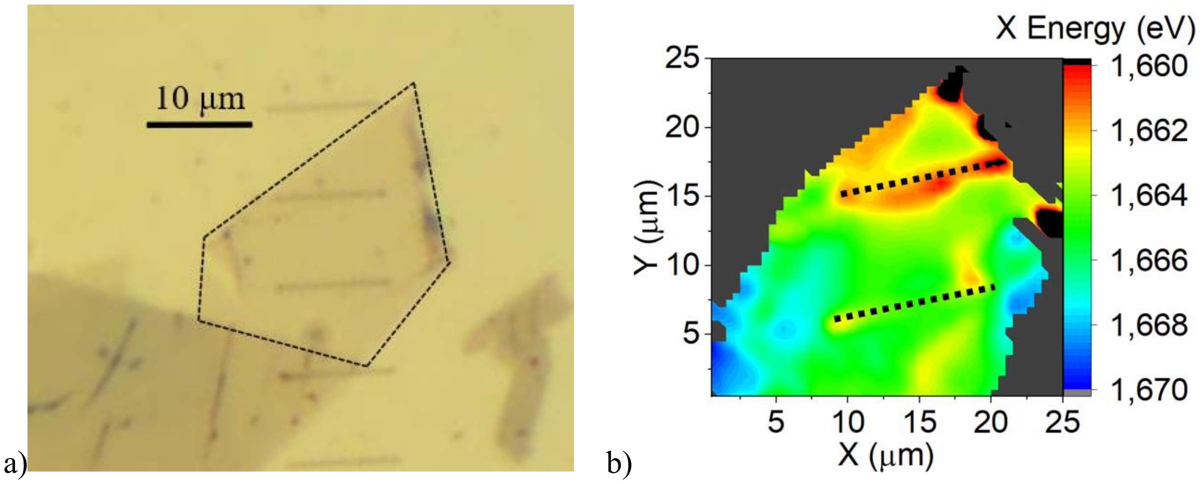

Figure 1. (a) Micrograph of the $MoSe_2$ flake deposited on GaAs nanomembranes. (b) PL map of the A exciton energy.

[1] Branny, A., Kumar, S., Proux, R. et al., Nat Commun 8, 15053 (2017).

P8

KPFM investigation of monolayer membranes based on $Mo_{1-x}W_xS_2$ alloys

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Recently, interest in atomically thin two-dimensional (2D) alloys has increased due to their promising applications in flexible electronic and optoelectronic devices. These alloys can be created by replacing atoms of metal or chalcogenides within the material's structure. Interestingly, this substitution process has minimal impact on the arrangement of atoms in the lattice but has notable effects on various properties such as optical, mechanical, and electrical characteristics. [1] Of particular significance are monolayer transition metal dichalcogenide (TMD) alloys, which represent a distinct class of 2D semiconductors. These materials offer unique opportunities for adjusting the energy band gap through alloying. Understanding how the electrical properties, including surface electric potential, are influenced by strain is essential for the advancement of sophisticated flexible electronics built on 2D TMDs. [2] We performed Kelvin force microscopy (KPFM) measurements on a series of monolayers of $Mo_{1-x}W_xS_2$ alloys on Au coated SiO_2 substrates. In addition, we performed Raman spectroscopy measurements to confirm the thickness of the membranes. The main objective of our work was to understand the influence of the substrate and material structure on the electrical properties of the studied membranes. In our work we confirm, that the work function of $Mo_xW_{1-x}S_2$ alloys change with increasing x. Our studies confirmed the influence of the substrate on the material and showed the existence of differences in surface potential between membranes made of different TMD materials and their alloys, suggesting variations in the conductivity of the materials.

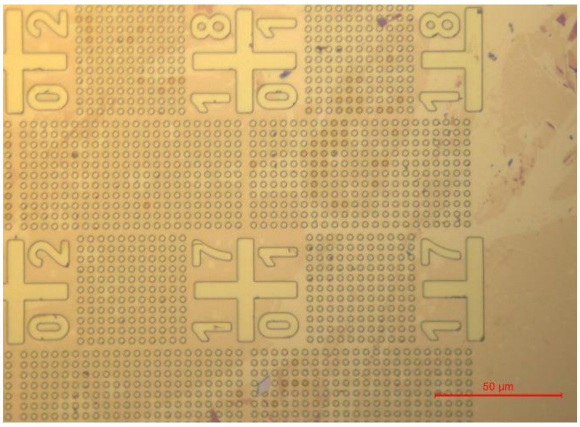

Figure 1. Optical image of the large-scale $Mo_xW_{1-x}S_2$ monolayer transferred on $Au/SiO_2/Si$ substrate with cavities.

[1] L. Ma, R. Chen, S. Dong, T. Yu *InfoMat*. **4**, 12310 (2022).
[2] Y. L. Chen, Z. Tian, X. Wang, N. Ran, C. Wang, A. Y. Cui, H. H. Lu, M. Zhang, Z. Y. Xue, Y. F. Mei, P. K. Chu, J. J. Liu, Z. G. Hu, Z. F. Di, *Adv. Mater*. **34**, 2201630 (2022)

P9

Unraveling the excitonic landscape in hybrid organic-inorganic two-dimensional silver chalcogenolates

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[3] *Massachusetts Institute of Technology, Cambridge, Massachusetts, United States*

In this work we use the optical spectroscopy techniques to investigate the optical properties of the compound AgSePh (“mithrene”), which belongs to the class of hybrid organic-inorganic metal-chalcogenolate materials. They sparked a great interest among the scientific community due to their unique optoelectronic properties. Mithrene is a direct-bandgap semiconductor, consisting of silver cations, selenium ions and organic ligands organized in a two-dimensional structure. Resulting spatial confinement greatly enhances the excitonic effects in this system, making it a convenient framework to study the exciton physics. Owing to the anisotropy of its 2D structure, mithrene displays strongly polarised light absorption and emission, giving way to even more potential applications.

We performed the polarisation-resolved photoluminescence and reflectance measurements at low temperatures (T = 5K) to probe the differently polarised excitonic states. In the reflectance spectra we have identified three previously reported excitonic transitions [1], named X_1, X_2 and X_3, each of them displaying a substructure and a linear polarisation dependence. Photoluminescence spectrum is rich, consisting of multiple narrow lines, within which we can identify the ones originating from the X_1 exciton recombination. Our results shed light onto the complex exciton manifold present in AgSePh, pointing out the need for further studies of this material, in order to understand the occurring phenomena and fully harness their application potential.

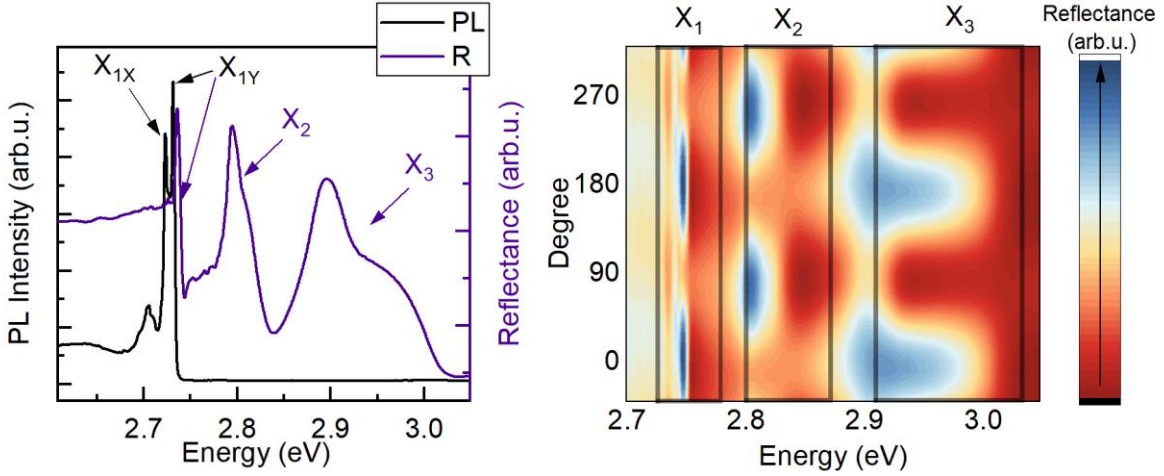

Figure 1. Left: Photoluminescence and reflectance spectra from AgSePh single crystal. Right: Dependence of the reflectance spectrum for AgSePh single crystal versus the polarisation angle. All measurements were done at T=5K.

[1] Lee, Woo Seok, et al. *ACS nano* 16.12 (2022): 20318-20328.

P10

Memristive Synapses for Neuromorphic Computing by CVD Grown Amorphous MoS$_2$

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Mimicking the human brain circuitry which is compose of synapses and neurons in order to overcome the ‘von-Neumann bottleneck’ present in conventional CMOS based architecture is an emerging area of research. A simple two terminal MIM structure based memory devices are attracting tremendous attention in the area of brain inspired Neuromorphic-Computing for the implementation of synapses and neurons which are commonly been implemented by using the oxide based or phase change material based devices. However this devices suffer from high variability and non-linear conductance change. Two-Dimensional (2D) material has gain the vast attention because of its atomic level scalability, flexibility, transparency, thermal stability [1], [2]. In this work we have realized the nonvolatile resistive switching using Au/Ti/MoS$_2$/Au/Cr device as shown in Figure 1(a). These devices exhibit the low cycle to cycle variability, multiple conductance states by applying the various compliance current. These synaptic devices are fabricated by using the amorphous multilayer MoS$_2$ which is synthesized by chemical vapor deposition process. These devices under study operates at low operating voltages for set/reset at <2/-2 V respectively with HRS to LRS ratio greater than 100 as shown in Figure 1(b-c). We believe the study on this devices will further enhance its application and usability in neuromorphic computing and logic circuitry.

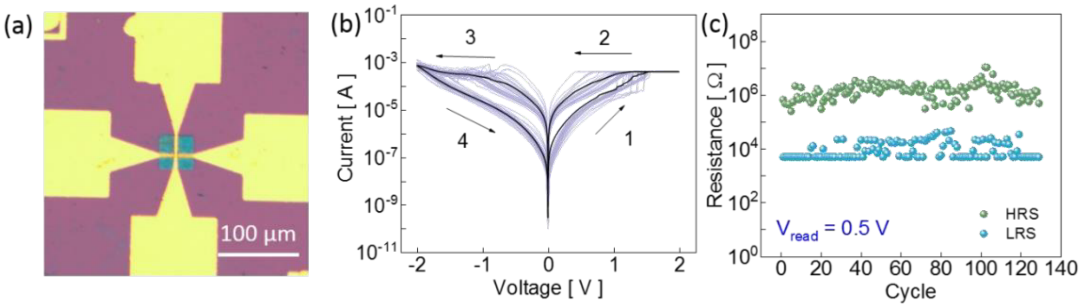

Figure 1. (a) Optical image of fabricated device Au/Ti/MoS$_2$/Au/Cr, (b) DC I-V Characterization at 100uA compliance, (c) HRS to LRS ratio read at 0.5 V.

[1] Saha, Puranjay, et al. *ACS nano* 18.1 (2023): 1137-1148.
[2] Krishnaprasad, Adithi, et al. *ACS nano* 16.2 (2022): 2866-2876.

P11

Improved Strain Engineering Of Atomically Thin MoS_2 By Polymer Encapsulation

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Controlling the band structure through strain engineering is an exciting avenue for tailoring optoelectronic properties of materials at the nanoscale [1]. However, in the case of 2D materials, weak van der Waals interactions can cause severe slippage between the material and substrate, dominating the bending or stretching processes and leading to inefficient strain transfer. Encapsulation of 2D materials is a promising technique to reduce this slippage, as well as to improve the transferable strain [2]. This approach shows increased strain transfer in many cases, although it can be difficult to accomplish for some encapsulating layers or materials [3]. In this work we report a comparative statistical study of the strain transfer modulation of MoS_2 flakes on polypropylene substrates, which have been encapsulated with three different solution–based polymers: polycarbonate (PC), poly(methyl methacrylate) (PMMA) and poly(vinyl formal) (Formvar). The flakes have been covered following a simple and cost–effective technique, in which the polymers in solution are spin-coated on the 2D material. Through micro-reflectance spectroscopy, we have observed a remarkable increase in strain gauge factors, which have been obtained by direct bending of the substrate, as well as by changing its temperature. In the first case, uniaxial strain is achieved, while in the second case biaxial strain is achieved due to the much higher thermal expansion coefficient of the polypropylene substrate compared to the MoS_2 flakes. The gauge factors seen for non-encapsulated monolayer and bilayer MoS_2 through uniaxial mechanical strain are ~30 $meV/\%$, while the ones achieved under the same conditions with PMMA or Formvar encapsulation lie around ~50 $meV/\%$. Maximum transferable strain before slippage also increased with encapsulation, achieving best results for Formvar and PMMA. An improve in the lifetime of MoS_2–based devices has also been observed. Finally, devices with Formvar encapsulation showed better photoresponse than their unencapsulated counterparts, as well as reduced dark current.

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[1] Castellanos-Gomez, A., Roldán, R., Cappelluti, E. *et al.* Local Strain Engineering in Atomically Thin MoS_2. *Nano Letters* **13**, 5361 (2013).
[2] Li, Z., Lv, Y., Ren, L. *et al.* Efficient strain modulation of 2D materials via polymer encapsulation. *Nat Commun* **11**, 1151 (2020).
[3] Carrascoso, F., Li, H., Obrero-Perez, J.M. *et al.* Improved strain engineering of 2D materials by adamantane plasma polymer encapsulation. *npj 2D Mater Appl* **7**, 24 (2023).

P12

Hybrid Devices Based on Transition Metal Oxides And van der Waals Materials for Tunneling Magnetic Junctions

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Advancements in the theory, synthesis and fabrication have led to the realization of 2D materials with ferroelectric or ferromagnetic properties, unlocking a realm where they can be seamlessly combined in heterostructures and finely tuned through mechanisms such as twisting, straining, or proximity effects [1][2].

In the first part of our study, we pursue two parallel research tracks. Firstly, following the work by Tan et al. [3], we study by magnetotransport measurements the ferromagnetic properties of thin-layered van der Waals metallic ferromagnet Fe_3GeTe_2 flakes on Si/SiO_2 substrates, revealing coercive fields around 0.6 T at 2 K. Results on magnetic anisotropy obtained by varying the direction of the magnetic field relative to the sample plane are shown, considering thin film demagnetization effects.

Concurrently, we characterize freestanding Barium Titanate (BTO) films (prepared in the Dept. of Materials Physics in the Universidad Complutense [4] and transferred onto Si/SiO2 substrates) using Piezoresponse Force Microscopy (PFM). Results will be presented on the stability of the PFM marks with time as well as the phenomenology encountered after laser Raman mapping on the polarized regions.

Our objective is to combine these two experimental lines by integrating these materials to create multiferroic magnetic tunnel junctions.

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[4] Puebla, S. *et al.* , *Nano Letters*, **22**,18, pp. 7457–7466 (2022).

P13

Lanthanum oxide halides as novel dielectrics for field-effect transistors

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Enhancing the fundamentals of field-effect transistors (FETs) involves improving their material properties. This can be achieved by replacing silicon and its oxides with 2D materials with superior characteristics. Lanthanum oxide halides (LaOX), a class of relatively unexplored 2D compounds, have recently been identified as layered dielectric materials[1], and for some of them high values of relative permittivity (κ) were theoretically predicted. Here, we studied the potential of LaOXs for 2D-FETs and compared three different compounds of this family: LaOCl, LaOBr and LaOI. Initially, a flux growth method inside an open corundum crucible was used to synthesize the materials. This way LaOXs were obtained in the form of a crystalline platelets up to several millimeter in diameter. Raman spectroscopy, XRD, SEM and EDS were used to characterize the resulting substances, confirming their desired composition. Next, the LaOCl, LaOBr and LaOI thin layers were produced by mechanical exfoliation and FETs were manufactured on prefabricated Si/SiO_2 substrates with either graphene or MoS_2 as a channel. The out-of-plane static dielectric constants were evaluated using double-gated graphene FET devices[2]. The results obtained demonstrate the dependence of κ values on different halogen atoms, showing the lowest value for LaOI and the highest for LaOCl. The potential to regulate the dielectric constant value by modifying the chemical composition of a group of compounds is an intriguing prospect. Thus, our results highlight its significant potential as a dielectric material for next-generation FETs.

[1] M. R. Osanloo, M. L. Van de Put, A. Saadat and W. G. Vandenberghe, *Nature communications* **2021**, *12*, 5051.
[2] A. Söll, E. Lopriore, A. K. Ottesen, J. Luxa, G. Pasquale, J. Sturala, F. Hájek, V. Jarý, D. Sedmidubský and K. Mosina, *arXiv preprint arXiv:2307.13431* **2023**.

P14

Integrated Computational Approach for the Treatment of Heterostructures of 2D Materials

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Heterostructure interfaces of two-dimensional (2D) materials enable the realization of advanced electronic functionalities at the nanoscale. The efficient computational *ab initio* modelling of these systems is, however, a challenge as it requires proper lattice matching of the component 2D sheets with minimal strain. This often results in large structures with hundreds to thousands of atoms. Moreover, the twist angle between the layers recently emerged as an important degree of freedom to control the properties of the resulting stacks.

Here, we utilize the newly developed Hetbuilder tool to automate the heterostructure cell construction based on coincidence lattice theory [1,2]. It is integrated with the AFLOW materials database and software [3,4] allowing for an efficient workflow (Fig.1) for the structure generation from the bulk parent systems. We benchmark the approach by reproducing a wide range of favorable theoretically and experimentally studied 2D heterostructures predicted by Koda *et al.* [1], finding all listed combinations as well as a few additional ones. We also perform *ab initio* calculations to study the electronic properties of "sandwiches" made by placing a layer of Al_2O_3 between two graphene sheets. The obtained band structures and density of states represent generally a superposition of the band structures and densities of states of the individual systems.

[1] D. S. Koda *et al.*, *J. Phys. Chem.* C **120**, 10895 (2016).
[2] https://zenodo.org/record/4721346.
[3] M. Esters *et al.*, *Comput. Mater. Sci.* **216**, 111808 (2023).
[4] C. Oses *et al.*, *Comput. Mater. Sci.* **217**, 111889 (2023).

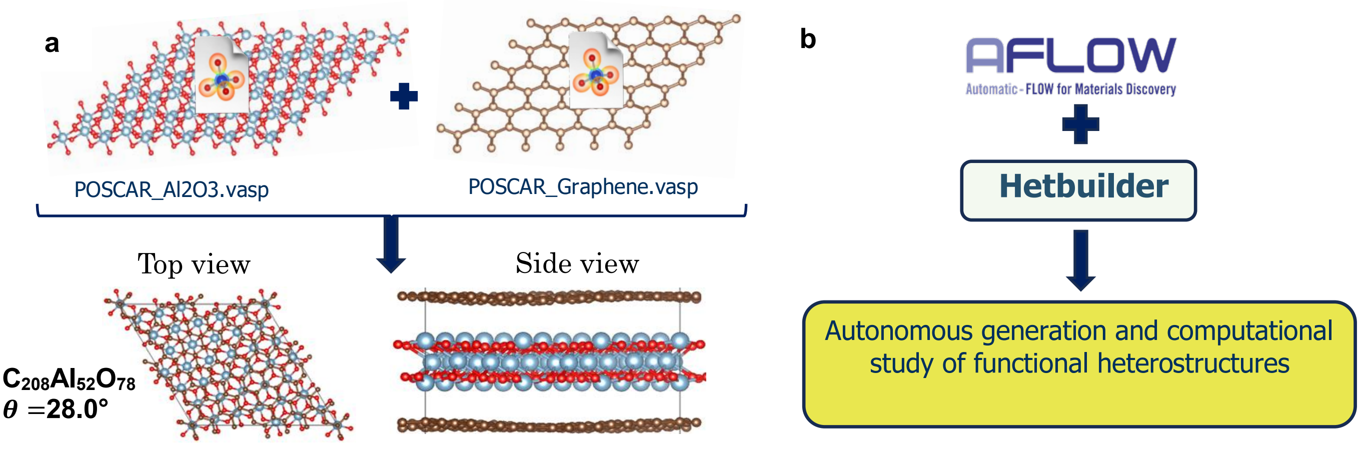

Fig.1 (**a**) Heterostructure generation with the Hetbuilder tool for the example of a sandwich structure out of Al_2O_3 and graphene. (**b**) Integrated workflow with the AFLOW database enabling the computational study of functional heterostructures.

P15

Beyond Graphene: Surface Functionalization of Germanane via Ge-H Activation

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Two-dimensional materials attract enormous attention across several scientific fields. The current demands in nano- and optoelectronics, semiconductors, or in catalysis have been accelerating the research process in the field of 2D materials. Among the 14th group 2D materials besides graphene and silicene, layered germanium represents a promising candidate for another class of materials, and its functionalization represents a way to tune its properties. Here, the exfoliation and functionalization of germanane surface is achieved *via* abstraction of hydrogen from Ge−H bond utilizing NaK equimolar alloy and its subsequent alkylation using *n*-alkyl halides or trifluoromethyl (CF_3) group containing benzyl halides. Composition of materials is confirmed by several methods including FT-IR, Raman, X-ray photoelectron, and energy-dispersive X-ray spectroscopy as well as X-ray powder diffraction. Scanning and transmission electron spectroscopy is used to reveal the layered morphology of functionalized germananes,[1] which can exhibit unique properties allowing them to be employed in sensing,[2] catalysis or as energy storage.[3]

[1] T. Hartman, J. Šturala, J. Luxa, Z. Sofer, *ACS Nano* **2020**, *14*, 7319-7327.
[2] T. Hartman, L. Valdman, J. Šturala, K. J. Sarkar, F. M. Oliveira, Z. Sofer, *Adv. Opt. Mater.* **2023**, *11*, 2300288.
[3] B. Wu, J. Šturala, M. Veselý, T. Hartman, E. Kovalska, D. Bouša, J. Luxa, J. Azadmanjiri, Z. Sofer, *Nanoscale Adv.* **2021**, *3*, 4440-4446.

P16

Comparison of the excitonic upconversion photoluminescence in MoSe2 monolayers with a different doping level

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Transition metal dichalcogenide monolayers represent unique platforms for studying both electronic and phononic interactions as well as intra- and intervalley exciton complexes [1]. The interaction between excitonic complexes in TMDC monolayers may be alternatively probed in upconversion (UPC) PL photoluminescence (PL) experiments. The excess energy required for the UPC process may be taken from phonons or resident electrons in the monolayer. Hence, the UPC PL provides information on both the energy spectra of the TMDCs as well as the scattering mechanism related to exciton–exciton, exciton–electron, and exciton–phonon interactions.

Here, we compare the UPC PL in an optically bright MoSe2 monolayer systems revealing different doping level. In hBN-encapsulated MoSe2 monolayers with a relatively weak electron concentration the UPC PL excitation reveals two pronounced resonances below the neutral 1s A-exciton (X). The resonance detected at an energy of about 25 meV below X coincides with the PL peak and binding energy of the singlet trion TS. The second resonance at −18 meV with respect to the exciton transition is attributed to the neutral biexciton (XX0). The mechanism of the exciton PL upconverted by the neutral biexciton is attributed to the interaction of the photocreated electrons at the K+ and K– valleys with zone-corner flexural acoustic ZA(K) phonons. The UPC of the X PL via the spin-singlet negative trion is assigned to a spin- and valley-conserving scattering process of the photocreated electron with the optical A1 phonon mode whose energy at the K valleys matches the energy difference between the singlet trion and the neutral exciton [1].

Interestingly, in uncapped MoSe2/hBN structures with the higher electron density the exciton UPC PL is hardly detected, whereas in hBN/MoSe2/graphene/hBN heterostructures, where the doping by resident charge carriers is completely neutralized and resultsin a vanishing trion emission, the UPC energy gain is about 17 meV and resonates with the energy of the zone-corner flexural acoustic ZA(K) phonon mode.

Our results extend the current discussion about interactions of electrons with both optical and acoustic phonons at the K valleys and their role in the upconversion of exciton emission in MoSe2 monolayers. We also provide further insights into resonant exciton–trion and exciton–biexciton couplings for optically exciting a 2D material within its nominal transparency range.

[1] J. Jadczak, J. Debus, J. Olejnik et al., J. Phys. Chem. Lett. 14, (39) 8702-8708 (2023).

P17

Magnetic State Control of Non-van der Waals 2D Materials by Hydrogenation

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Controlling the magnetic state of 2D materials is a key enabler for spintronics. Especially in the novel class of non-van der Waals 2D compounds – materials derived from non-layered bulk counterparts – promising (surface) magnetic properties were outlined in recent years [1,2]. Utilising data-mining and autonomous density functional theory calculations, we demonstrate the modification of magnetic properties of these materials by hydrogen passivation [3]. Employing extensive stability assessments, including checks for supercell reconstructions and phonon calculations, four stable candidates are outlined. The magnetic configurations are tuned to states with flipped and enhanced moments, which we rationalize by analysing Bader charges and density of states. For 2D $CdTiO_3$ – a diamagnetic compound in the pristine case – we observe an onset of ferromagnetism with a mean-field Curie temperature of ~10K and in-plane magnetic anisotropy upon hydrogenation. Further investigation of the magnetization density in both pristine and passivated systems, as exemplified in Figure 1, provides a detailed analysis of modified local spin symmetries and the emergence of ferromagnetism. Our results suggest that selective surface passivation is a powerful tool for tailoring magnetic properties of nanomaterials, such as non-vdW 2D compounds.

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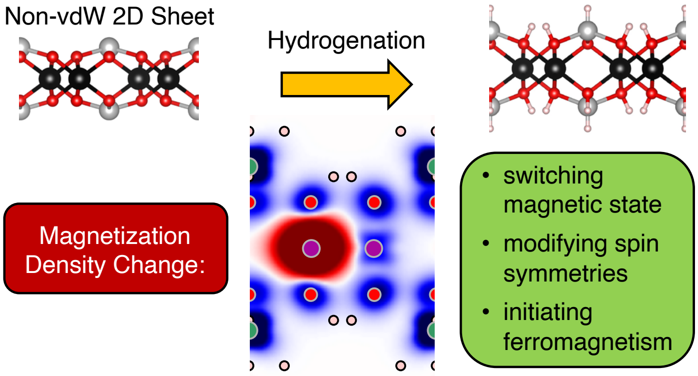

Figure 1. Schematic representation of the structural and magnetic modifications upon hydrogenation for a representative non-vdW 2D layer.

P18

Mn-doped WSe$_2$ as effective electrocatalyst for hydrogen evolution reaction and as anode in lithium-ion batteries

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The rising global energy demand, driven by population growth and increasing energy consumption, presents a significant challenge. With fossil fuel reserves dwindling, there's a growing focus on renewable energy sources.[1,2] However, the high cost and limited availability of lithium resources pose challenges for lithium-ion batteries (LIBs).[1] Meanwhile, electrochemical water splitting for hydrogen production shows promise, but the cost and availability of current electrocatalysts hinder widespread adoption.[2] Therefore, exploring alternative materials for these applications is crucial.

In this context, transition metal dichalcogenides (TMDs) have received considerable attention as electrocatalysts in hydrogen evolution reaction (HER) but also as anodes for LIB.[1,2] Tungsten diselenide (WSe$_2$), although less researched among TMDs, presents certain advantages.[3,4] For instance, heavier chalcogens generally provide enhanced electrical conductivity, a critical characteristic for energy-related uses. Additionally, tungsten is more economical and environmentally friendly than molybdenum. Incorporating atoms into TMDs enhances their electrocatalytic activity at defective sites by forming covalent bonds within the material. This process generates new electronic states crucial for electrocatalytic properties but often involves complex and high-temperature procedures like chemical vapor deposition or pyrolysis. Therefore, we achieved the successful integration of Manganese (Mn) into WSe$_2$, creating Mn-doped WSe$_2$, using a straightforward hydrothermal approach.[5] This novel material exhibited outstanding electrocatalytic activity for the HER and demonstrated superior performance as an anode for LIB.

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P19

Mechanism of WS_2 Nanotube Formation revealed by *in situ/ex situ* Imaging

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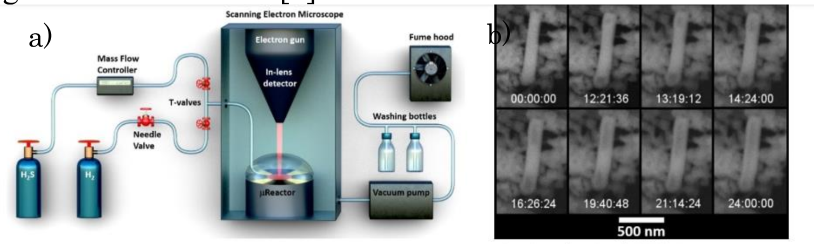
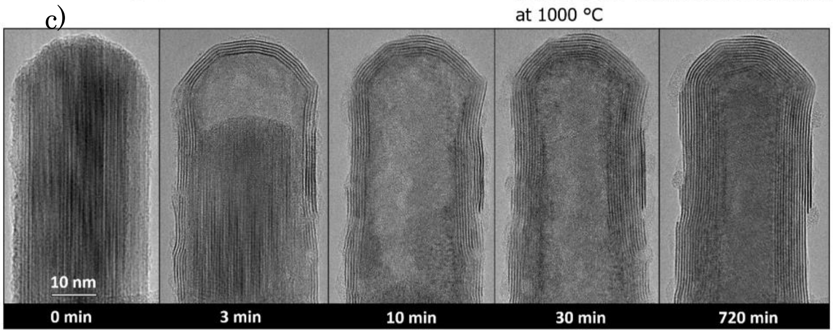
Metal dichalcogenide nanotubes, and in particular those made of WS_2, are known for over 30 years and have been investigated extensively. Synthesis of macroscopic amounts of such nanotubes has been demonstrated in the past. The tungsten suboxide $W_{18}O_{49}$ nanowhiskers are converted to WS_2 nanotubes by a high-temperature reaction in the stream of a gaseous mixture of H_2S and H_2.

Scanning and transmission electron microscopy (SEM and TEM) play a crucial role in the structural characterization of nanomaterials. Various tools related to electron microscopy are available and under development for a deep understanding of reactions and nanostructures. The μReactor technology allows in-situ observation of high-temperature heterogeneous reactions within a scanning electron microscope in a low-pressure atmosphere (up to 500 Pa). For the current work, the expedient SEM with a fitted mReactor was further developed for in-situ observation of sulfidation reactions. The coupling of in situ sulfidation in SEM and sequential ex situ TEM, both on the Micro Electromechanical System (MEMS) chip, revealed the mechanism of the WS_2 nanotube formation. Subsequent to the presentation of the modified μReactor and the experimental results, the growth mechanism of the nanotubes is discussed in light of the new growth environment. [1]



Scheme of the SEM with the fitted μReactor for in-situ studying of sulfidation reactions

In-situ obtained SEM image sequence of the $W_{18}O_{49}$ nanowhisker sulfidation (H_2+H_2S) and WS_2 nanotube formation at 1000 °C



Ex-situ obtained TEM images sequence of the $W_{18}O_{49}$ nanowhisker sulfidation at 1000 °C

a) Scheme of μReactor SEM dedicated to sulfidation reactions b) sequence of *in situ* obtained images showing WS_2 nanotube formation upon sulfidation of $W_{18}O_{49}$ nanowhisker c) *ex situ* TEM obtained sequential analysis of WS_2 nanotube formation progression at selected times oft he reaction observed on the selected nascent nanotube

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P20

Submillimeter-Long WS_2 Nanotubes: The Pathway to Inorganic Buckypaper

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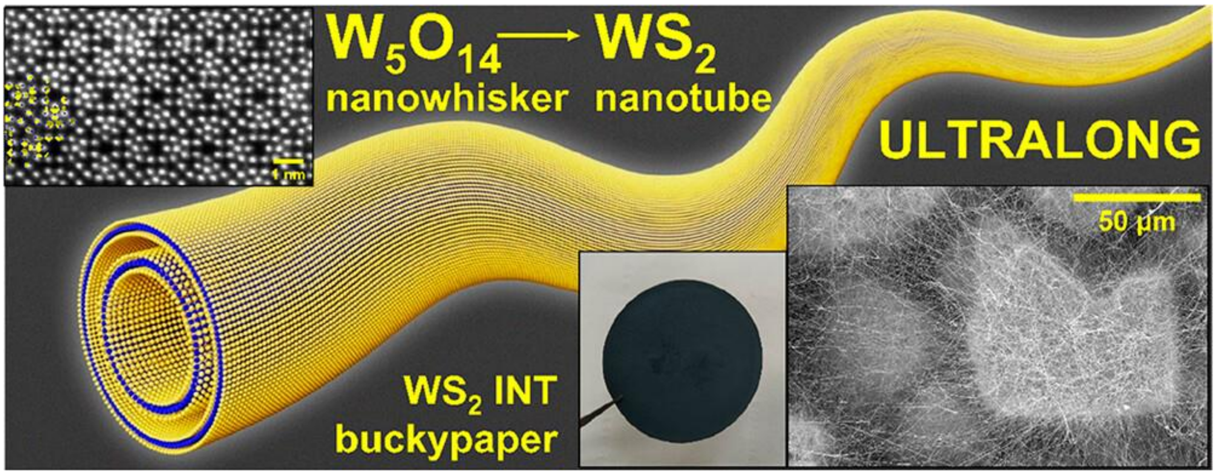
WS_2 nanotubes present many new technologies under development, including reinforced biocompatible polymers, membranes, photovoltaic-based memories, ferroelectric devices, etc. These technologies depend on the aspect ratio (length/diameter) of the nanotubes, which was limited to 100 or so. A new synthetic technique is presented, resulting in WS_2 nanotubes a few hundred micrometers long and diameters below 50 nm (aspect ratios of 2000–5000) in high yields. The preliminary investigation into the mechanistic aspects of the two-step synthesis reveals that W_5O_{14} nanowhisker intermediates are formed in the first step of the reaction instead of the ubiquitous $W_{18}O_{49}$ nanowhiskers used in the previous syntheses. The electrical and photoluminescence properties of the long nanotubes were studied. WS_2 nanotube-based paper-like material was prepared via a wet-laying process, which could not be realized with the 10 μm long WS_2 nanotubes. Ultrafiltration of gold nanoparticles using the nanotube-paper membrane was demonstrated. [1]



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P21

The influence of electrical contacts to MoS_2 monolayer on its optical properties

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Semiconducting transition metal dichalcogenides (TMDCs) present new possibilities for designing novel electronic devices, including light-emitting diodes, which require an efficient contacting scheme. However, the latter is challenging for TMDCs, mostly due to the typically high Schottky barrier (SB) formed between a metal and a semiconductor (SC). In theory, the barrier height is given by a difference between the work function of the metal and the electron affinity of the SC [1], but in practice, the Fermi level at the metal/SC interface is typically pinned as a result of metal-induced gap states. A recent report by Shen et al. [2] presents the possibility of obtaining ohmic contacts between semimetalic bismuth and a semiconducting TMDC layer. Due to the near-zero density of states at the Fermi level of the semimetal, the gap states are sufficiently suppressed, making possible to obtain low-resistance ohmic contacts to TMDC.

In this study, we compare electrical properties of Bi and Au contacts to a MoS_2 monolayer, additionally investigating the extent to which the type and quality of the electrical contact affects the photoluminescence (PL) spectrum of the sample. In the case of Au contacts, the exfoliated MoS_2 layer was deposited on previously evaporated Ti/Au pads and then ironed with a tip of an AFM microscope in a contact mode. In the case of Bi contacts, the MoS_2 layer was deposited on a Si/SiO_2 substrate and then Bi/Au contacts were evaporated. The I-V curves of both samples were measured in the temperature range from 300 K to 2 K. The Au contacts show clear Schottky characteristics, with the majority of them not conducting below 100 K, despite the calculated Schottky barrier being lower than that typically reported in the literature [3]. In contrast, the Bi contacts exhibit ohmic behaviour from room temperature down to 80 K. While the ohmic behaviour is lost below this temperature, the contacts still conduct current down to 2 K. The contact and channel resistances in 280 K were calculated using the transfer length method, with the result that the contact resistance was found to be negligibly small compared to the channel resistance (equal 46.6 $k\Omega/\mu m$).

Both samples were investigated by means of PL spectroscopy. The spectrum of the sample with Bi contacts was found to be unusual for a MoS_2 monolayer and to be significantly different from the spectrum of the sample with Au contacts. To gain further insight, we measured microphotoluminescence maps for both samples, with all contacts grounded. Each spectrum was integrated in two ranges - around 1.9 eV (trion) and around 1.8 eV (defect). It is evident that grounding the contacts has a more pronounced effect in the case of the sample with Bi (ohmic) contacts, which suggests a correlation between the type and quality of contacts and the observed luminescence spectrum.

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P22

Exploring the Optical and Magnetic Properties of a Two-Dimensional Magnetic Semiconductor - CrSBr

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Magnetic semiconductors are garnering significant interest in both technological and theoretical fields due to the interplay between their electronic structure and magnetism, which facilitates spintronic and magnetoelectric phenomena. Such properties allow for applications in spin injection, the development of magneto resistive devices, and direct-read magnetic memory technologies. Additionally, if a magnetic semiconductor possesses a direct band gap or undergoes optically allowed crystal field transitions, it may exhibit photoluminescence, broadening its utility to include light-emitting and processing technologies. The rules governing optical transitions in these materials are shaped by their overall symmetry, which is a composite of the crystal lattice's symmetry, the symmetry of electronic orbitals, and the spin/magnetic order inherent in the material. Therefore, controlling the magnetic order, for instance, through temperature adjustments or external magnetic fields, could significantly affect the optical properties of a magnetic semiconductor, offering novel avenues for manipulating material characteristics. [1]

CrSBr is a two-dimensional orthorhombic layered material known for its unique electronic and magnetic properties. It features strong ferromagnetic intralayer interactions and antiferromagnetic interlayer coupling, making it an A-type antiferromagnet. CrSBr exhibits a direct band-gap of around 1.5 eV and is known for its highly anisotropic electronic and optical properties. This material has shown significant potential for applications in spintronics and magnetoelectronics due to its ability to maintain magnetic properties even in monolayer form. The magnetic order in CrSBr can be controlled through temperature or external magnetic fields, impacting its optical properties and offering new avenues for material control.

In the experimental approach undertaken on the sample, a series of detailed photoluminescence and reflectance measurements were conducted, with a particular focus on their variation with respect to polarization, temperature, and the influence of high magnetic fields. The study also extended to evaluating the dependency of photoluminescence characteristics on the excitation power and wavelength, offering a more nuanced understanding of the sample's optical response under various excitation conditions.

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P23

Rapid synthesis of hBN on commercial Ni foils by pre-annealing and CVD in ultra-high vacuum

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Two-dimensional hexagonal boron nitride (hBN) is a subject of significant interest due to its unique mechanical strength, thermal stability, and chemical inertness [1]. Challenging synthesis of large-area single-crystalline hBN can be tackled via chemical vapor deposition (CVD), particularly in ultra-high vacuum (UHV-CVD), thus offering controllability and insight into the growth mechanisms which can be exploited for further advancement of hBN growth.

The growth of hBN, primarily on transition metal substrates like Cu and Ni, has shown success on commercial polycrystalline Cu [2] and Ni [3] foils. Notably, focus has shifted to nickel substrates due to the improved control over growth and the number of hBN layers [4]. Our research involves UHV-CVD growth of hBN on recrystallized Ni foils. In particular, as-received 50 µm thick Ni foil is annealed (for cca. 3 minutes) using electron bombardment heating in the UHV chamber, followed by SEM and AFM characterization. The annealed foil is then returned to the UHV for hBN synthesis, and subjected to ex situ microscopic analysis of the morphological changes and the fabricated 2D material. We find that well-defined crystal domains and terraces form on the annealed Ni foil's surface, and as such are suitable for the epitaxial growth of hBN films, as confirmed by the distinctive triangular shape of hBN islands (see Fig. 1). Future work aims to optimize synthesis conditions to enlarge hBN domains, crucial for meeting applicative requirements. Also, efficient transfer methods of hBN onto desired substrates, such as Si-wafers or 2D material heterostacks, will be developed in which cheap Ni foil substrates can be readily sacrificed. Our results showcase how affordable metal foils can be quickly and effectively transformed to well-defined substrates suitable for the scalable growth of 2D materials, all in highly controllable UHV environment.

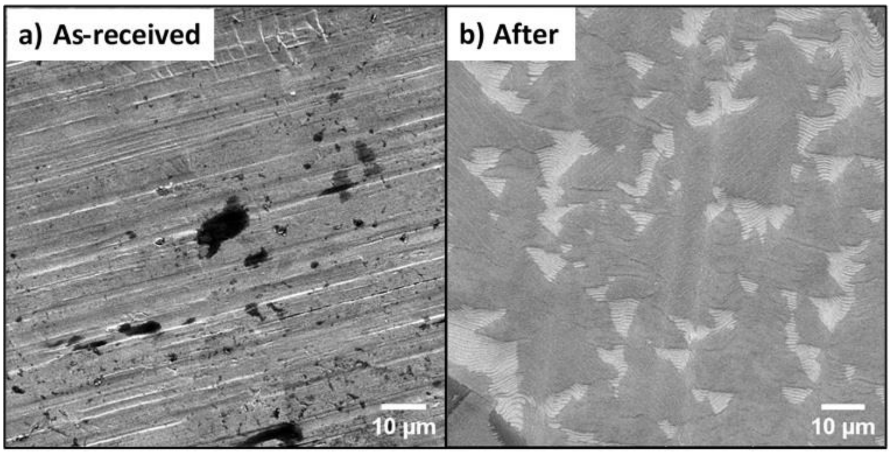

Figure 1: SEM images of: a) as-received Ni foil, and b) Ni foil after annealing in ultra-high vacuum and CVD growth with borazine as a precursor, showcasing distinct terraces and epitaxially grown hBN films.

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P24

Improving Chemisensor Reliability using Machine Learning

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Ion-sensitive field-effect transistors (ISFETs) have emerged as a promising technology due to their remarkable precision that comes in conjunction with a highly scalable design [1,2]. However, the reliability of ISFETs is impeded by various non-ideal factors including cycle-to-cycle, sensor-to-sensor, and chip-to-chip variations. In this study, we leverage the capabilities of machine learning algorithms to mitigate the impact of these variations, using non-functionalized graphene-based ISFETs as a testbed. We utilize pH-sensing as a benchmark to illustrate the advantages of integrating ML algorithms with ISFET sensors before demonstrating the ability of the sensing platform to discern instances of food fraud, food spoilage, and food safety concerns. The cross-sectional schematic of a graphene-based ISFET is depicted in **Fig. 1a**. **Fig. 1b** shows the transfer characteristics of seven ISFETs across two chips measured for 25 cycles in pH buffer solutions. We extracted 20 figures of merit (FOMs) that are directly linked to the transport properties of graphene-based ISFETs and demonstrate that pH sensitivity experiences a significant reduction when incorporating cycle-to-cycle, sensor-to-sensor, and chip-to-chip variations. First, the performance of the k-NN algorithm was evaluated over all possible combinations of input FOMs for a given input dimensionality. The accuracy statistics are displayed in **Fig. 1c**. These results are then compared to those obtained through the training of a convolutional neural network (CNN). To explain the performance of the CNN trained on ISFET characteristics, we extensively evaluate the feature space of the trained CNN model through the utilization of SHAP (SHapley Additive exPlanations) [3] features and compare regions of interest obtained from maximally activated nodes to human-derived FOMs. SHAP features of a correctly classified ISFET measurement at each pH level are shown in **Fig. 1d**.

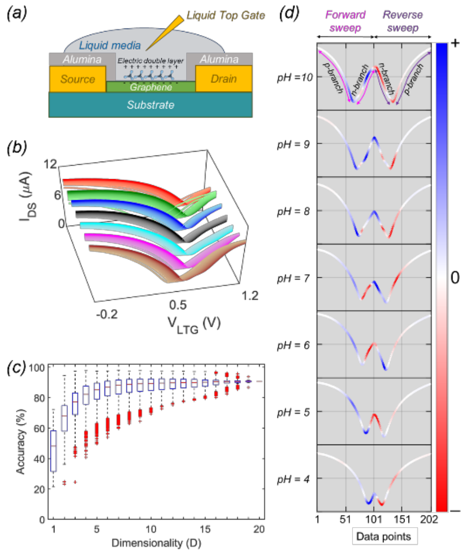

Figure 1.

Next, we broaden the application scope of ML-assisted graphene ISFETs to address key challenges in the food industry by measuring common food products to create food adulteration and food authentication datasets. The food adulteration dataset comprises whole milk adulterated with different percentages of water while the food authentication datasets contain subgroups of related food products, i.e., several types of sodas, milks, and coffee blends. Finally, we demonstrate that the ML- assisted graphene ISFETs can be deployed as a solution to assess the freshness of consumer food products by extracting juices from four different fruits (orange, grape, watermelon, and pineapple) and monitoring them with graphene-based ISFETs over four consecutive days as they gradually perish. We utilize a multi-output model to simultaneously predict juice identity and freshness.

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P25

Exploring the Optoelectronic Properties of CsPbBr3 Nanowires

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Metal-halide perovskites (MHPs) have brought a revolution in the field of photovoltaics due to their simple production process and unique optoelectronic properties. They are not only used in solar cells but also in light-emitting diodes, photodetectors, and lasers. Simultaneously they constitute an interesting material system for fundamental photo-physics investigation in bulk and quantum-confined regimes. So far the investigation of perovskite nanostructures has been dominated by the studies of their 0D [1] and 2D [2] forms however quasi-1D nanowires can also be obtained [3]. These nanowires can be used as potential components in various applications, showing properties such as low threshold lasing and polarity-dependent photodetection. Moreover, the $CsPbBr_3$ nanowires, are more stable than bulk forms.

Here we show our investigation of the optical properties of stable, single-crystal $CsPbBr_3$ nanowires grown by surface-guided chemical vapor deposition [3], which reflect the symmetry or morphology of their sapphire substrates. These horizontal $CsPbBr_3$ nanowires, guided on surfaces, present unusually large size-dependent emission blue shifts, significantly beyond the quantum confinement regime, related to substantial and uniform lattice distortion due to heteroepitaxial strain and lattice relaxation. Such wires provide a great opportunity to study the continuous evolution of the band-structure parameters due to strain in metal halide perovskites.

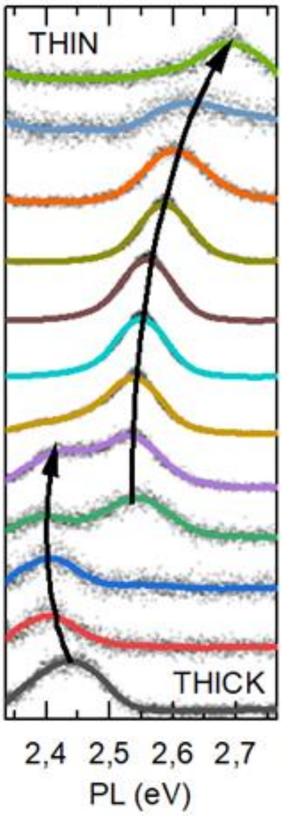

Fig. 1. Normalized PL spectra of photoluminescence emission taken at different points along the nanowire

We will show detailed photoluminescence, time-resolved photoluminescence and reflectance characterization of $CsPbB_{r3}$ nanowires characterized by the strong change of their optical response along the wire length. We will show how the strain modulation impacts the structural phase transition of $CsPbBr_3$ nanowires and how the 1D form affects the polarization of the emitted light.

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P26

Photo- versus electroluminescence of the WSe_2 monolayer: a comparative study

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Photoluminescence (PL) and electroluminescence (EL) are essentially similar types of spontaneous emission of light from an excited state of a material. The key difference comes from the way of carriers excitation. While the PL emission emerges after excitation of the material using a laser light, the EL appears as a result of an electric current passed through the material. Comparison of these two experiments in monolayers (MLs) of semiconducting transition metal dichalcogenides (S-TMDs), *e.g.* WSe_2 ML, may develop our knowledge about them for their potential applications in optoelectronic devices.

In this work, we investigate the optical response of a light-emitting tunnelling structure based on a WSe_2 ML as an active emission material. The stacking sequence for the sample is: the central WSe_2 ML is encapsulated between two thin hexagonal BN (hBN) flakes being tunnelling barriers, which are embedded between two graphene layers serving as electrodes. The Figure shows the results of the PL and EL measurements at low temperature (T=4.2 K). The obtained PL spectrum composed of a series of emission lines with the highest energy peak related to the neutral exciton (X) is in agreement with the analogous PL spectra of the WSe_2 ML close to the neutrality point, reported in the literature [1]. In contrast, shapes EL spectra exhibit the completely different from the PL response, as well as from each other, while the sign of the applied voltage is reversed. The first difference, *i.e.* between the PL and EL, can be understood in terms of different types of excitation, it means photon versus tunnelling current. Furthermore, the applied voltage needed to observe the EL signal is much larger than the electronic band gap of the ML (~1.9 eV) [2] suggesting additional parasitic processes, which substantially reduce the tunnelling current, and hence the intensity of the EL. The EL disparity reveals different thicknesses of to hBN barriers, leading the unintentional doping the WSe_2 ML due to various numbers of tunnelling electrons and holes. We identify that under positive and negative applied voltages the WSe_2 ML is correspondingly doped with holes (*p*-type) and electrons (*n*-type).

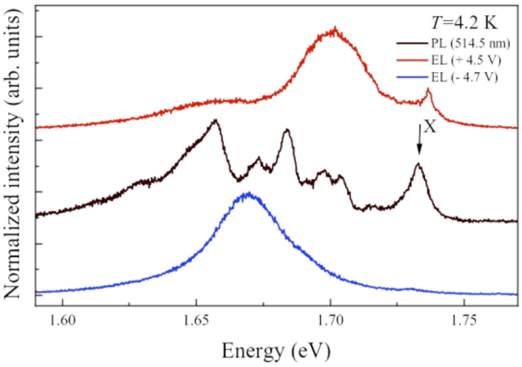

Figure: PL and EL spectra of WSe_2 ML. The spectra are normalized to the maximum intensity and shifted vertically for clarity.

Our results of comparative investigations give us important information of the potential applications of S-TMD MLs in optoelectronic devices.

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The antibacterial and photocatalytic activity of versatile lacquer coatings enhanced with MXene and MBene phases

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Global concerns about infectious diseases spreading through contaminated surfaces have become increasingly alarming. Environments with high levels of surface contamination, such as intensive care units, are particularly at risk of bacterial cross-transmission, including the transmission of multidrug-resistant strains. Antimicrobial coatings offer a promising strategy to hinder the colonization of pathogenic bacteria on various surfaces. The flexibility and convenience of these methods make them stand out, outperforming current solutions. Originating from Martin Jones' 2012 patent, these coatings utilize lacquer dispersions containing synthetic resins. The incorporation of engineered nanoparticles is considered as a strategic approach to enhance their biocidal properties. Nevertheless, their limited efficacy and susceptibility to invasive bacterial species highlight the need for more robust solutions [1].

To address this challenge, the utilization of 2D nanomaterials with unique characteristics, such as Mxenes and MBenes, has been proposed. These are solid crystals composed of transition metal carbides, nitrides, carbonitrides, and borides, derived from their parental MAX and MAB phases. Such materials exhibit a distinctive accordion-like morphology and can be further separated into individual nanoflakes [2]. Following synthesis, MXenes and MBenes showcase distinctive optical and photocatalytic properties. These properties inspire scientists to explore their potential in the development of antimicrobial coatings. When integrated into coating, their antimicrobial mechanism involves the release of active ionic species or the photocatalytic generation of reactive oxygen species through light absorption.

Our study [1] aimed to explore the impact of introducing $Ti_3C_2T_x$ MXene, obtained through the HF/TMAOH approach, into lacquer formulations. The stability of the resulting colloidal lacquer dispersions, refining the MXene content to minimize nanoflake agglomeration in the final formulation was evaluated. Transparent plastic sheets underwent coating with the optimized lacquer dispersions, and examination was conducted on their morphology, distribution of $Ti_3C_2T_x$ MXene, and optical properties. We noted a favorable shift in the band gap, coupled with efficient light absorption. These distinctive characteristics facilitated a self-cleaning mechanism, allowing for the removal of adsorbed coloring contaminant upon exposure to light. The coatings also displayed biostatic properties against both *Escherichia coli* and *Staphylococcus aureus*. Further exposure to simulated daylight revealed nearly 100% effectiveness against both bacterial strains, showcasing remarkable self-sterilizing capabilities. Moreover, we recommended a future research direction involving MBenes synthesized using an HCl/H_2O_2 method and presented our findings from the optical properties analysis of the MBene-enriched coatings. To summary, our investigation successfully verified the multifunctionality of the developed lacquer coatings through the incorporation of MXene.

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P28

Distinguishable Optical Signature in Bilayer AA and AB'_{XY} Stacked ReS$_2$: A Comprehensive Investigation

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Polymorphism, stacking order, and twist angle-driven manipulation of physical, optical, and electronic properties in TMDCs are of the utmost interest to the scientific community recently. ReS$_2$ is a relatively less explored member of the TMDC family with regard to its staking sequence-dependent properties. [1], [2] Herein, we report the distinction between AA and AB'_{XY} bilayer ReS$_2$ based on optical properties. Two different kinds of stacking AA (0° orientation) and AB'_{XY} (layer 180° rotation and 1/10th shift along the 'b' axis) have been confirmed by cross-sectional HRTEM. A very fast-hand observation is the optical contrast (OC), where AA stacks show high OC compared to AB'_{XY} stacks due to the change in refractive index, which is theoretically investigated by absorption spectroscopy. A significant change is observed in the Raman mode, especially the I-III peak separation, **Table 1**, verified by theoretical phonon band analysis. AA stacked layers do not show any SHG due to the preservation of inversion symmetry. On the contrary, AB'_{XY} stakes show the SHG based on the even layer where the symmetry breaks **Fig [1]**. DFT calculation of band structure shows the difference in band gap for ReS$_2$ stacking. Low-temperature PL measurements of AA and AB'_{XY} stacked BL shows the difference in exciton energy of ~ 40 meV, which supports theoretical outcomes. We believe this polytypism in ReS$_2$ will further enhance the manipulation of physical properties based on the stacking sequence.

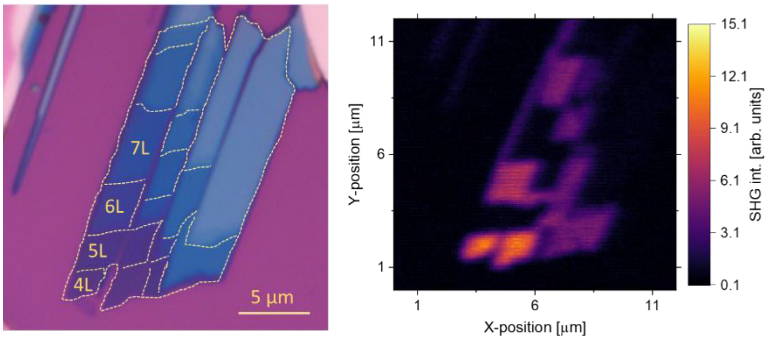

Figure 1. OM and SHG images.

Table 1. Distinct features of AA and AB'_{XY} ReS$_2$

Stacking [2L]	OC (%)	Raman shift	HRTEM	SHG	PL
AA	High (14%)	Δω ~ 14 cm^{-1}	0°	No SHG	Band-gap 1.57 eV
AB'_{XY}	Low (11%)	Δω ~ 18 cm^{-1}	180°	Even-layer SHG	Band-gap 1.61 eV

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P29

Upconversion photoluminescence of a defect-bound exciton in hBN- encapsulated MoS$_2$ monolayers

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Recent advances in the elaboration of high-quality TMDCs monolayers surrounded by hBN have provided in-depth insights into the excitonic complexes properties as well as the exciton-exciton and exciton-phonon interactions revealed by optical spectroscopy experiments [1]. However, TMDCs monolayers prepared by mechanical exfoliation can have a native defect density of about 10^{13} cm^{-2} [2], which usually reduces the performance of their opto-electronic properties. These atomic defects mainly comprise chalcogen vacancies, which can form gap states and alter doping. Hence, in most TMDCs monolayers the broad sub-gap emission appears at low temperatures about several hundred meV below the neutral exciton X. This sub-gap luminescence is often called L-band and typically its intensity grows for increasing density of point defects and can be observed over a wide range of temperatures, even up to room temperatures [3].

Here, we demonstrate upconversion (UPC) photoluminescence (PL) of a defect-localized exciton X_L in hBN/MoS$_2$/hBN structures with a high energy gain of about 292 meV at 7 K. The upconverted PL is observed only for samples in which the prominent X_L line dominates the neutral exciton X in low-temperature PL spectra. Furthermore, we evaluate the UPC PL dependence on changes in the excitation energy, incident laser power and temperature. The intensity of upconverted X_L transition decreases with decreasing laser excitation energy, reflecting the shape of the lower energy flank of the X_L PL line, whereas its dependence on the laser power is sub-linear. We propose that the energy gain required in the UPC of the defect-bound exciton PL originates from an electron Auger recombination between in-gap defect defect states introduced by chalcogen vacancies.

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P30

Extremely high excitonic g-factors in $MoWSe_2$ monolayer alloy

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Monolayers (MLs) of semiconducting transition metal dichalcogenides (S-TMDs), *e.g.* $MoSe_2$ and WSe_2, are direct bandgap semiconductors characterized by very interesting optical and electronic properties. S-TMD alloys have emerged as materials with tuneable electronic structures and valley polarizations [1].

In this work, we investigate the properties of monolayers (ML) of $MoWSe_2$ alloys encapsulated in hexagonal boron nitride (hBN) by reflectance contrast (RC) and photoluminescence (PL) experiments performed in external out-of-plane magnetic fields ($B_\perp$) up to 30 T. We examined MLs with different ratio of Mo/W atoms: 0.46/0.54, 0.55/0.45, and 0.66/0.34, as well as the $MoSe_2$ and WSe_2 MLs.

Under applied magnetic fields, the bright neutral exciton (X) resonances in S-TMD MLs split into two circularly polarised components ($\sigma^\pm$) due to the Zeeman effect [2]. The $\sigma^\pm$ energy separation can be expressed as $\Delta E(B_\perp) = E_{\sigma^+} - E_{\sigma^-} = g\mu_B B_\perp$, where g denotes the effective g-factor of the neutral exciton and μ_B is the Bohr magneton. Using this formula, we extracted g-factors values for X transitions for all investigated samples.

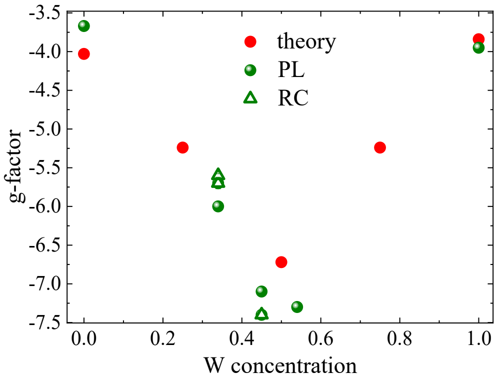

Figure 1. The g-factors for neutral exciton (X) as a function of tungsten (W) concentration in $MoWSe_2$ MLs. Green and red points correspond to the values of g-factors extracted from experimental data and theoretical calculations, respectively.

As can be seen in the Fig. 1, the g-factors of the X transitions extracted for the $MoSe_2$ and WSe_2 MLs are of the order of -3.7 and -4, respectively. These values are in agreement with the ones reported in the literature [3]. Surprisingly, the corresponding g-factors of the X resonances found in the MLs of the $MoWSe_2$ alloys exhibit much larger magnitudes. They increase from around the aforementioned -4, through around -6 for the $M_{0.66}W_{0.34}Se_2$ ML, reaching almost -7.5 for the MLs characterized by the about 50/50 ratio of the Mo/W atoms. Moreover, the experimentally obtained values are confirmed by theoretical calculations using density functional theory (DFT), which follow exactly the same trend. The large values of the found g-factors cannot be understood in terms of orbital, valley and spin contributions within few-band models, but come from particular arrangements of bands and their mixing, which can only be captured by DFT calculations.

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P31

Native point defects in transition metal dichalcogenides MX_2 (M = Mo or W; X = S, Se, or Te): experimental verification of theoretical prediction

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Transition metal dichalcogenides (TMDs), specifically two-dimensional (2D) MX_2 (M = Mo or W; X = S, Se, or Te), are considered to be promising for a variety of electronic, photonic, energy and sensing device applications that are more efficient than cutting edge silicon based devices. In this work, we present experimental and theoretical studies of native point defects in TMDs. The deep-level defects were revealed and their charge transition levels were measured by means of deep level transient spectroscopy (DLTS). The DLTS results agreed well with the state-of-the-art computational predictions, made by density functional theory (DFT), using the optimized functional, electrostatic correction, and band alignment. The very good agreement of experimental and computational results validated the computational approach and allowed for identification of the origin of experimentally revealed defect levels. We found that the chalcogen vacancy is the most stable defect in bulk MX_2, which creates the $0/-1$ charge transition inside the band gap and that the selection of transition metal has only little effect on the position of the $0/-1$ charge transition. Verified DFT approach has been then used to calculate the charge transition levels of defects in monolayer 2D MX_2, which are experimentally challenging to be measured directly by DLTS. This is because of their atomic-scale thickness, which excludes the existence of a sufficient width of the depletion region to be modulated by voltage pulses through the vertical Schottky diode or p-n junction during measurements. By comparing the bulk and 2D TMDs data, we find that reduction of dimensionality of TMDs to 2D has a significant impact on defect properties, their formation energies and chemical trends of their charge transition levels. For example, unlike the bulk systems where the metal vacancies have many transition levels inside the band gap, in the 2D systems the metal vacancies create only a single transition level inside the band gap. This finding may explain observed differences in optical properties of 2D TMDs synthesized with different methods and lays foundation for future developments of more efficient TMD-based applications.

P32

Probing Interlayer Interactions in MoS₂ Nanoscrolls: Insights from Photoluminescence Spectroscopy and Structural Study

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Transition metal dichalcogenide nanoscrolls (NS) have emerged as promising nanostructures with intriguing photoluminescence (PL), despite their multilayered structure, challenging conventional understanding. In this study [1], we look into the interlayer interactions within NS to unravel this mystery. Our investigation reveals that the traditional strained multilayer description fails to explain the observed PL signals. We attribute the reduction of interlayer interactions in NS to two key factors: (1) a symmetry-broken mixed stacking order between adjacent layers induced by misalignment and (2) a high degree of inhomogeneity in the strain landscape stemming from the unique Archimedean spiral-like geometry characterized by positive eccentricity. Experimental evidence from transmission electron microscopy, field emission scanning electron microscopy and atomic force microscopy supports these findings. By employing low-temperature PL spectroscopy, we scrutinize the behaviour of K-point excitons in multilayered MoS_2 NS, shedding light on the effects of reduced interlayer interactions. We discuss the implications of these findings on exciton-phonon coupling, exciton energy and exciton oscillator strength. This provides valuable insights into the distinctive properties of NS, advancing fundamental understanding of interlayer interactions in NS and paving the way for the rational design of NS-based optoelectronic devices.

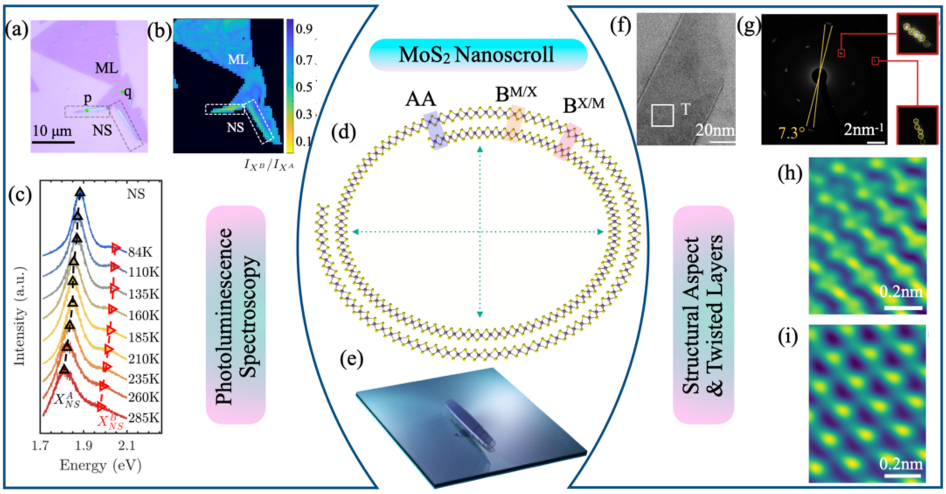

Figure 1 (a) Image of Partially scrolled MoS2. (b) Mapping of B-, A- excitonic peak intensity ratio. (c) Temperature-dependent PL spectra of NS. (d) Schematic showing cross-section of NS. (e) Schematic showing a NS. (f) TEM image of a NS tip. (g) SAED in region T of (f) showing twisted layers of NS. (h-i) Symmetry broken moiré-like stacking arrangements of NS layers.

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P33

Molecular functionalization of atomically thin phototransistors

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Atomically thin semiconducting materials are promising for the ultraminiaturization of electronic components, flexible devices and transparent optoelectronic actuators [1]. Due to the reduced out-of-place dimension, these materials are very sensitive to the presence of physisorbed species [2]. This offers new possibilities for sensing [3] but it can also be used for enhancing and tailoring the electronic and optoelectronic properties of such materials and devices. In this work, we have fabricated phototransistors based on a single layer of 2D semiconductors such as MoS_2 (Figure 1a). First, it is characterized the effect of air exposure on the electrical performance of the devices due to the oxygen and water molecules present in the ambient (Figure 1b), and strategies to mitigate these effects. Then, photoactive molecules are deposited on the devices, where it is observed a similar effect on the electronic properties, but in this case gives rise to an increase of the photoresponse, which can be tuned by band engineering, being the enhancement exciton dependent (Figure 1c). Finally, the material is functionalized with a molecular bond to Pd-nanolayers to extend the photoresponse of the devices to the infrared for broadband applications (Figure 1d). It defines a path for a new generation of molecular scale transistors and photodetectors with enriched performance.

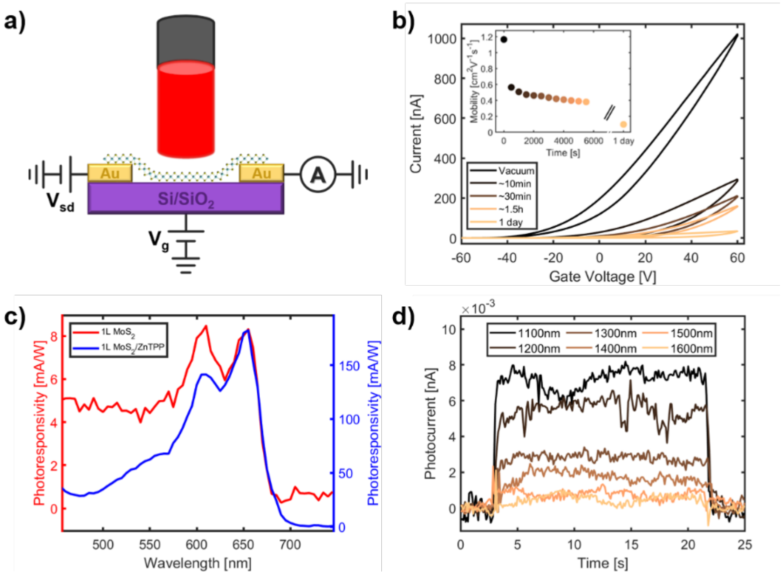

Figure 1. (a) Schematic of the measurements of a single-layer MoS_2 phototransistor. (b) Selection of transfer curves recorded after annealing in vacuum and after venting the system at several time points. (inset) Time dependence of the mobility in vacuum and after venting the system for several time points. (c) Wavelength dependence of the photoresponsivity for a single-layer MoS_2 device before (red) and after (blue) functionalization by deposition of ZnTPP molecules. (d) Superimposed photocurrent pulses from 1100 nm to 1600 nm excitation wavelength with on-times of 20 s and at 1 V bias voltage for a single-layer MoS_2 device functionalized with Pd-nanosheets.

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P34

Roll-to-Roll Exfoliation for Anisotropic Films of 2D Materials

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This document provides instructions for preparing an abstract for “MIRSENS5” and is written in the format according to the guidelines given below.

The recent development of roll-to-roll high-throughput exfoliation technique for the production of high-density van der Waals materials has opened a world of possibilities for scaling the fabrication of electronic devices based on 2D materials [1]. This method has shown to produce large-area films composed of interconnected flakes of van der Waals materials, yielding superior device performance compared to other low-cost, high-yield 2D material production methods like liquid-phase exfoliation. In addition to its scalability, we have explored the potential of leveraging the unidirectional exfoliation orientation that this method offers to exfoliate materials with highly anisotropic structures, such as black phosphorus (BP) or germanium sulfide. Since this exfoliation method tends to preserve the orientation of our materials, we are able to fabricate polarizers or photodetectors that respond based on the incident light angle.

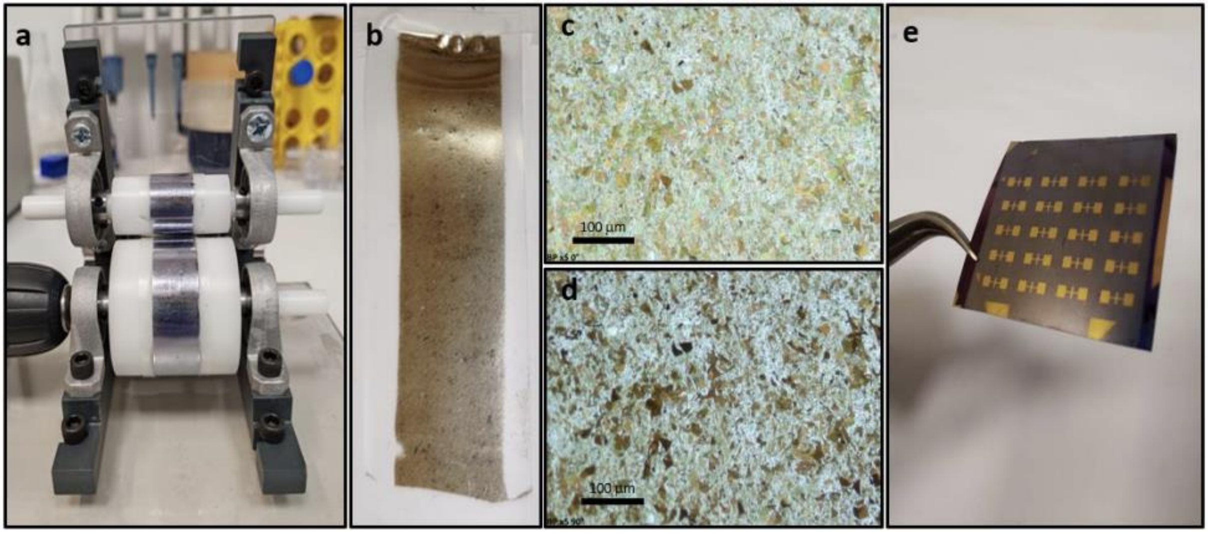

Figure 1 a) Picture of the massive parallel exfoliation device after the exfoliation of the crystal of BP. b) Picture of the sample obtained after exfoliation. c) Picture of the tape under the microscope, illuminated with light polarized at a 0-degree angle. d) Picture of the tape under the microscope, illuminated with light polarized at a 90-degree angle. e) Fabrication of devices on a silicon oxide wafer by thermal evaporation to analyze their optical and electrical properties.

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P35

Optical d-d transitions in magnetic transition metal oxychlorides

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Two-dimensional (2D) magnetism, for many years were considered impossible to obtain due to strong thermal fluctuations [1]. That changed with experimental observation of magnetic order in 2D CrI_3 [2]. From that moment 2D magnets draw interest, especially in cases such as topology studies or detection and control of spin. Therefore exploring magnetic layered van der Waals (vdW) materials is crucial for understanding fundamental difference beetwen 2D and 3D ferromagnetism (FM) and antiferromagnetism (AFM) [3,4].

The transition metal oxychlorides (MOCl) are vdW semiconducting crystals exhibiting magnetic properties. In contrast to most of vdW magnets, which have a honeycomb structure with high lattice symmetry, MOCl have orthorombic structure characterized by higher anisotropy. It gives opportunity for more potential applications by addition of another degree of freedom in magnetism modulation [5].

In this work we present various spectroscopic measurements, such as transmission, reflection and photoacustic spectrocopy (PAS), of optical transitions in TiOCl, VOCl, CrOCl and FeOCl crystals. Experimental methods were supported by density functional theory (DFT) calculations. Optical absorption measurements along with PAS shows several absorption features in wide range from 1 to 4 eV. Comparison with DFT calculations allowed us to assigned them to specific band to band transitions.

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P36

PtX_2/graphene (X = S/Se/Te) hybrids with enhanced catalytic performance

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Two-dimensional (2D) materials have been proven effective in energy applications such as energy storage (supercapacitors, batteries) and catalysis. Among them, Pt-based Transition Metal Dichalcogenides (TMDs) have been reported to have promising performance in Hydrogen Evolution Reaction (HER) [1]. However, their use remains limited mainly due to the high cost of using Pt. In this work, we will fabricate graphene-based hybrid nanostructures with different Pt-based TMDs. Graphene hybrids are also potential candidates for HER [2], and through their use, the amount of Pt can be reduced while tuning physical properties and catalytic behavior. Density functional theory calculations imply a strong interaction between the graphene and PtX_2 (X = S, Se, Te) heterostructures, while a band-gap opening is observed in all cases. The hybrid nanostructures were fabricated with liquid-phase exfoliation, which is a cost-effective procedure that also offers the possibility of industrial scalability [3]. Transmission and scanning-transmission electron microscopy (TEM/STEM) observations revealed the morphological features of the exfoliated flakes, with graphene to be decorated with the Pt-based TMDs. STEM-EDX mapping confirmed the presence of all involved elements in all cases. UV-vis and Raman spectroscopies revealed the optical properties of the hybrid systems, which are modified concerning the individual materials. Finally, the performance of 2D inks in HER was evaluated, while a comparative study was conducted on the effect of different chalcogen on the hybrid structures.

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P37

Water-soluble WS_2 Transient Photodetector for Sustainable Electronics

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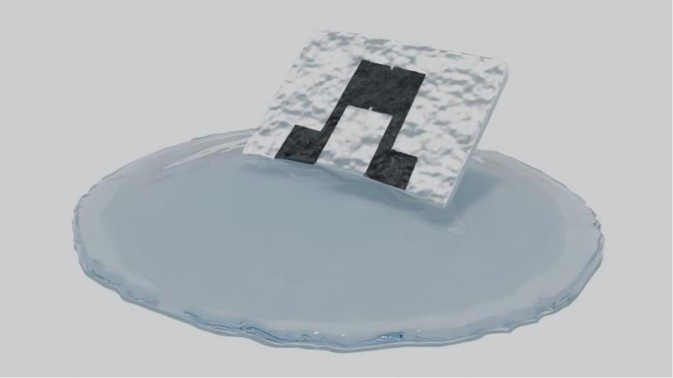
The rapid development of technology has led to a significant increase in electronic device production. However, this growth also brings forth the challenge of electronic waste (e-waste). To overcome this challenge, transient electronics with the capability of disintegrating or disappearing after stable operation have attracted widespread attention in recent years. Controlled disintegration of such systems without the need for harsh solvents is a step toward realizing green and sustainable electronics. Transient electronics have a wide range of potential applications as biomedical implants, environmental sensors, and hardware-secured devices.

In this work, we demonstrated a dissolvable ecofriendly flexible photodetector using an abraded WS_2 on a soluble paper substrate. The whole device can physically disappear in water solutions in a period of ~60s and be recycled by vacuum filtering while it shows a photoresponsivity of ~176 µA W-1 under ambient conditions. This work demonstrates our photodetector yields zero waste with a minimum impact on the environment, which is very useful for the development of the sustainability of our planet.



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P38

Fabrication of Thin Film Field-Effect Transistors via Langmuir–Schaefer deposition

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The advancement of semiconductor microscale devices exploiting two-dimensional (2D) van der Waals (vdW) heterostructures elevates the contemporary fabrication methodologies for field-effect transistors (FETs) [1, 2]. The integration of a range of 2D layered materials into the FET structural matrix yields considerable adaptability in engineering diverse transistors employing a variety of fabrication approaches. To satisfy the scalable fabrication requirements, solution-phase printing has emerged in the fabrication of electronic devices. The technologies such as 3D printing, inkjet printing, and aerosol inkjet printing are used to fabricate solution-processed electronics utilizing semiconducting inks of 2D layered transition metal chalcogenides (TMCs). However, these methods do not feasibly suit the deposition of large-area film. 3D printing, for instance, is designed for the rapid production of relatively thick films, while inkjet printing is more suitable for the slow production of uniform thin films with stringent requirements for the inks used [3]. In contrast, the deposition protocols of Langmuir–Schaefer for semiconducting inks exhibit promise in fabricating vertically stacked heterostructures, displaying successful outcomes in the creation of expansive, conductive TMCs-based nanosheet films and transistors [4, 5]. In this work, we present the method for the development of thin film field-effect transistors using the inks of 2D materials and mask-based optical lithography. We investigate the semiconducting inks prepared via liquid phase exfoliation of graphene and electrochemical exfoliation of semiconductors (MoS_2, WSe_2) the Langmuir–Schaefer technique for the deposition of inks as channel materials for thin film field-effect transistors.

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Earth-abundant minerals as dielectrics for 2D heterostructures

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The field of two-dimensional (2D) dielectrics has been dominated by hexagonal boron nitride (hBN) due to its inherent flatness and lack of surface dangling bonds. These characteristics give it superior interfacing capabilities to other 2D materials, improving device performance and stability compared to conventional bulk dielectrics. [1]

However, thicker layers of hBN are needed to prevent electric breakdown, which in combination with its weak relative permittivity (ε_r) reduces the effective field present at the semiconductor. In addressing these shortcomings, we explore the potential of phyllosilicates such as mica and talc as alternative dielectric materials. These earth-abundant minerals exhibit promising properties, including a substantial increase in ε_r compared to hBN, and could be synthesized for very large-scale integration as well. [2–6]

Moreover, the possibility for elemental substitution in phyllosilicates in general and the presence of interlayer ions in micas present pathways for functionalizing the dielectric-semiconductor interface through mechanisms such as charge transfer doping, and harnessing hysteresis for innovative computing applications. [1, 7]

In this study, we present our findings on deterministically stamped 2D field-effect transistors fabricated using various 2D dielectric / 2D semiconductor combinations, demonstrating charge transfer doping and the resultant changes in device characteristics when 2D phyllosilicates are used as gate dielectrics. Electrical characterization of these devices is conducted across a range of temperatures, supplemented by Kelvin probe force microscopy (KPFM) analysis to provide insights into the local electronic properties.

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Mo_2B_2 MBene as Robust Photocatalyst for Organic Compounds Decomposition

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Innovative two-dimensional (2D) nanomaterials represent groundbreaking structures with outstanding optical features, including superior light absorption and the transition from direct to indirect bandgap, along with their hydrophilic properties and diverse surface terminations. These distinctive attributes make them ideal candidates for serving as photocatalysts, particularly in environmental engineering applications and the decomposition of organic dyes. Within the realm of 2D materials, researchers specifically recognize transition metal carbides, nitrides, and carbonitrides known as MXenes and post-MXene materials that contain boron in their structure instead of carbon and nitrogen called MBenes [1].

Unfortunately, wet-chemical etching and delamination of the MoAlB phase are still challenging. Herein, it is overcome by processing MoAlB for 24, 48, and 72 h with an aqueous HCl/H_2O_2 solution to obtain single flakes of material. The process of etching and delamination over time produces separate single-to-few layered 48-MBene flakes. We then analyzed the optical properties of Mo_2B_2 MBene, observing superior outcomes.

Following this, we carried out the photocatalysis process with the innovative catalyst Mo_2B_2 MBene after 48 h of synthesis. The novel catalyst exhibited over 90% efficiency in decomposing the model organic dye methylene blue under UV and simulated white light irradiation, and approximately 50% efficiency in decomposing a commercial textile dye blend after 30 min of irradiation. With a direct band gap of approximately 1.22 eV, and 0.22 eV for an indirect band gap, the 48-MBene also demonstrated tunable activity towards maximum photocatalysis efficiency with all tested visible light ranges (violet, blue, cyan, green, amber, and red). Mechanistic analysis revealed high reactive oxygen species (ROS) evolution activity by the functional groups on its surface and the high activity of charge carriers. Post-process analysis confirmed no changes in the properties, morphology, or structure of the nanostructure.

Furthermore, the catalyst was successfully regenerated and reused with excellent efficiency. Thus, our novel catalyst represents an environmentally friendly solution with significant potential for MBene-enabled industries [2].

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Photoemission study of $SnSe_2$ van der Waals crystal – the influence of native defects on the electronic properties

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$SnSe_2$ crystal is a van der Waals semiconductor with great potential for applications in photocatalysis and thermoelectric conversion, as well as in two-dimensional optoelectronics and nonlinear optics [1-3]. According to DFT calculations, it exhibit indirect band gap in the near infrared spectral range [4]. The fundamental properties of $SnSe_2$ and its efficiency in certain applications are strongly influenced by the presence of native donor defects, pushing the Fermi level into the conduction band. In our study, we investigate the electronic band structure of $SnSe_2$ by angle resolved photoemission spectroscpy (ARPES). In the ARPES maps, along with the valence band dispersion, we were able to detect signal originating from the conduction band valley populated by the electrons from ionized defects. The obtained results allowed us to directly determine the Fermi level posioton and the electronic band gap, as well as experimentally observe the characteristic flat dispersìon of the valence band. Additionaly, the optical absorption spectroscopy revealed the presence of the Burstein-Moss effect (an effective blueshift of the fundamental absorpion edge due to occupation of the lowest conduction band states). The experimental findings are supported by *ab initio* calculations of the electronic band structure and native defect formation energies, suggesting which defects most likely contribute to the observed phenomena.

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Interlayer Energy Transfer in WS_2-hBN-MoS_2 Heterostructure

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Heterostructures (HSs) made by the vertical stacking of van der Waals monolayers (1Ls) have shown great potential in next-generation opto/electronic device applications [1]. Interlayer energy transfer (ET) is one of the main photocarrier relaxation pathways in these materials. In type-II transition metal dichalcogenides (TMDs) HS, long range ET happens *via* the dipole-dipole coupling (Förster type) [2]. To investigate this further, we studied a HS made by the 1Ls of tungsten disulfide (WS_2) and molybdenum disulfide (MoS_2), with hexagonal boron nitride (hBN) as a charge-blocking interlayer (optical micrograph in Figure a), using differential reflection contrast (RC), photoluminescence (PL), and photoluminescence excitation (PLE) spectroscopy. We find that there is significant WS_2 PL enhancement from the HS area when we excite with 2.13eV photon (Figure b). This enhancement is due to the resonance between the excitation energy, the B excitonic level of MoS_2 and (close to) the optical bandgap of WS_2, which facilitates an efficient ET from the MoS_2 to WS_2 layer at room temperature (300 K) under vacuum conditions. Our preliminary results show great promise for studying the interlayer ET process from a *lower-to-higher* bandgap material.

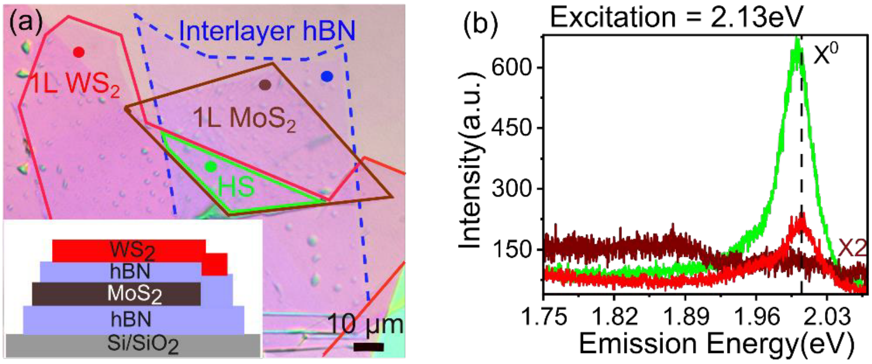

Figure: *(a) Optical image of the sample with a schematic illustration of the cross-sectional view of the HS as an inset. (b) PL spectra from the three areas of the sample with an excitation energy of 2.13eV (here, dashed vertical line indicates the position of the neutral exciton(X^0) of WS_2; ×2 represent the multiplication factor of the intensity of MoS_2), which clearly shows the enhancement in the intensity of the WS_2 neutral exciton in the HS region compared to the 1L of WS_2. This confirms the energy transfer from MoS_2 to WS_2 at room temperature.*

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Manipulation of hybrid interlayer excitons in 2D materials

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Structures consisting of two stacked TMDC monolayers exhibit interlayer excitons, where the electron and hole are spatially separated in the two different layers. These interlayer excitons themselves have comparatively low oscillator strength, which may limit their use in the context of polaritonics [1].

However, in systems of two layers of TMDCs, the aforementioned interlayer exciton can couple to an intralayer exciton, leading to the formation of a hybrid interlayer exciton. Here, the electron in one layer interacts with a hole tunneling between both layers [2]. This configuration has an out-of-plane dipole moment and a high oscillator strength. The degeneration of the dipole orientation can be lifted by an external electric field, leading to a splitting into two different states. These two states can be attributed to the dipole moments parallel and antiparallel to the external electric field [3,4,5].

Furthermore, these hybrid interlayer excitons show a stronger interaction with each other compared to the A exciton. Thus, by increasing the exciton density, the blueshift of the hybrid interlayer exciton exceeds the blueshift of the A exciton [6,7].

We study the exciton resonances by introducing a high exciton density while applying an out-of-plane electric field and observe an enhanced blueshift of the hybrid interlayer exciton compared to the A exciton providing information on the interaction of the different excitons.

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Machine-Learning Accelerated Quantum Correction to Hydrogen Diffusion in Between Layers of Transition Metal Dichalcogenides

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In groundbreaking experiments by Geim's group, layered materials such as h-BN and MoS_2 have demonstrated a remarkable ability to let hydrogen isotopes pass between their layers.[1] Further theoretical analysis uncovered that it is hydrogen atoms, rather than ions, that travel between these layers, aided by shearing modes within the material.[2] In our earlier research, we revealed that hydrogen transport is significantly affected by stacking configurations and stoichiometry, leading to variations in diffusivity.[3] When it comes to lighter atoms like hydrogen, quantum effects become critical. Yet, previous theoretical studies relying on well-tempered metadynamics (WTMetaD) used a classical approach under the Born-Oppenheimer approximation.

In this study, we investigate the nuclear component quantum mechanically using Path-Integral Molecular Dynamics (PIMD). This combination with metadynamics improves with quantum corrections to the classical model. Although PIMD requires significantly more computational power than classical molecular dynamics, machine-learning potentials (MLPs) offer a solution, improving future calculations.

Here, we first explore how diffusivity changes in classical WTMetaD, both with and without MLPs, using models trained on our previous results[3] and PIMD trajectories. Next, by employing MLPs within PIMD, we directly compare diffusivity to its classical counterpart, understanding the quantum nature of hydrogen transport within layers of 2D materials.

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Excitonic g-factors in van der Waals structures beyond simple models

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The shifts of optical peaks energies under external magnetic field, quantified by effective *g*-factors, provide a deep insight into electronic and excitonic structures of two-dimensional materials. A recently developed first-principles-based method for calculation of *g*-factors, including bands-summation formula, yields excellent agreement with experiments for intralayer excitons in monolayer (1L) transition metal dichalcogenides (TMDCs), interlayer excitons in TMDCs heterobilayers, as well as larger excitonic complexes in doped 1L TMDCs [1,2]. The last case corroborates the accuracy of the method for evaluation of single bands *g*-factors. Here we present more advanced cases which are beyond the possibilities of simplistic models with separate spin, atomic orbital and valley contributions. We explain the reduction of *g*-factors measured in $MoSe_2$/WS_2 moiré heterobilayer by inclusion of exciton *g*-factor's dispersion and spatial confinement in moiré potential [3]. Inclusion of excitonic wavefunctions calculated by model Bethe-Salpeter equation enables us to understand the measured excitonic state dependence of *g*-factors in 1L and homobilayer TMDCs [4,5]. We analyze the influence of biaxial strain on 1L TMDs, finding a large strain dependence of excitonic *g*-factors, with significant spin-mixing effects [6]. The calculated trends of direct and indirect excitons *g*-factors in WS_2 micro-bubbles allow us to explain the strain-induced exciton hybridization in WS_2 monolayers unveiled by magnetooptical measurements [7]. We investigate a new class of hexagonal 2D materials with formula MSi_2Z_4 (M: Mo, W; Z: N, P, As, Sb), which are isosymmetric to 1L TMDCs. We find a new set of circularly polarized excitonic transitions with high binding energies and large positive g-factors [8]. All these new observations cannot be understood by means of simple models that were employed previously.

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P46

Signatures of interlayer character in electric and magnetic fields

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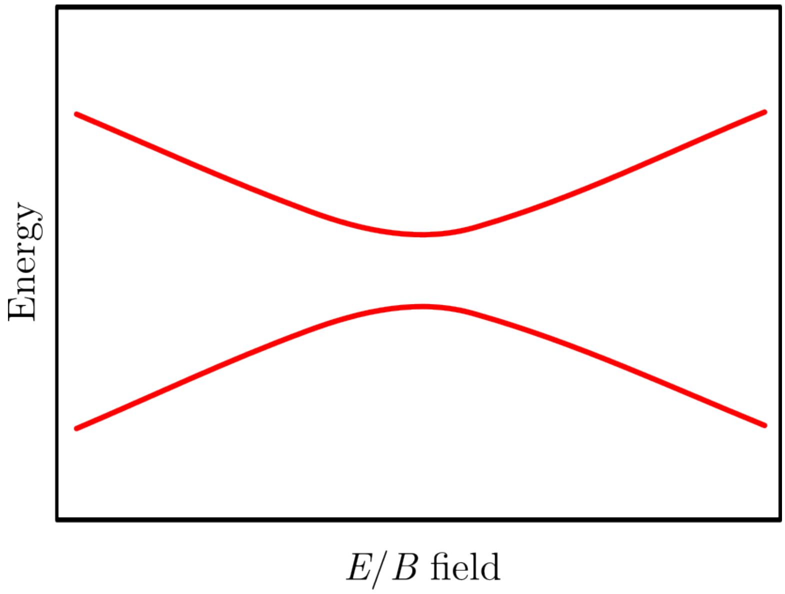
Over the past years, there has been tremendous effort and progress in the field of two-dimensional (2D) materials. A particularly fascinating topic is the coupling of different layers. This coupling is present in heterostructures between two different materials [1], but can also be found between the same layers up to bulk semiconductors such as $MoTe_2$ [2].
Here we report on the interlayer coupling that can occur in mulitlayer structures. First, we discuss the coupling of a trilayer heterostructure of MoS_2 and WS_2. In contrast to bilayers, the coupling may lead to quadrupolar excitons. These can be clearly identified by the quadratic response of the corresponding excitons in our GW/BSE calculations in electric fields. In the second example, we report our studies of bulk CrSBr [3]. In a magnetic field the lowest bright excitations of the antiferromagnetically coupled CrSBr shift quadratically. Our calculations reveal the symmetry forbidden dark excitons and the increasing interlayer character. We develop a minimal model to explains this spin-dependent coupling. Despite its simplicity, the proposed model is generally applicable to any coupled 2D magnet.



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Signal Amplification and Overcoming of Saturation Effect in Photoacoustic Spectroscopy

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Photoacoustic spectroscopy (PAS) is a powerful technique to investigate semiconducting samples and determine some of their basic properties e.g., energy gap [1], thermal conductivity [2] and thermal diffusivity [1, 3]. Most importantly, the PAS technique does not require special preparation of samples. Using this method, it is possible to measure samples that are difficult to study by conventional absorption/transmission techniques due to high scattering of light, opaqueness, or the state of the sample, i.e., powdered/liquid form [4 – 6]. These advantages are because, in PAS, sound is detected instead of light. Moreover, this also means that the sensitivity of this method does not vary with the spectral range due to the requirements of using different photodetectors. However, just like any measurement technique, PAS also has limitations. One of them is signal saturation, which causes difficulties in investigating some of the properties of studied samples. Hence, one of the goals is to improve the sensitivity of PAS. Due to above, in this work we focus on enhancing photoacoustic (PA) signal intensity in a non-complex way, which does not require changing any part of a measurement setup. We show how to improve sensitivity in this technique, mainly by manipulating the sample volume and its environment. Moreover, we show a simple model that we proposed to describe and explain obtained results in thermal terms. Additionally, we present how to correctly determine an energy gap based on the PA measurement since there is no consensus in this aspect, and so far, in many articles this parameter is obtained in different ways depending on investigated materials.

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Interplay between structure and magnetism in MPS_4

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Magnetic van der Waals materials, such as transition metal phosphorus chalcogenides MPS_3 and MPS_4 (M = Mn, Fe, Co, Ni), offer potential for spintronic and optoelectronic applications due to their wide band gaps (1.2 - 3.5 eV) [1] and efficient light absorption. Both belong to the C2/m space group but differ in magnetic ordering: MPS_3 maintains antiferromagnetic (AFM) ordering [1], while $CrPS_4$ shifts from AFM to ferromagnetic (FM) in the monolayer limit [2]. However, the mechanisms involving ligand field theory and exchange interactions are still unclear, necessitating further research on the magnetic states in $FePS_4$, $CoPS_4$, $MnPS_4$, and $NiPS_4$, and their instability factors.

We studied the stability and electronic properties of the MPS4 family using DFT, focusing on magnetic properties. VASP with PAW, PBE+D3, optB86-vdW functionals, and the SCAN functional were employed with the GGA+U approach with Dudarev formalism. Analysis was done using a Heisenberg model derived using TB2J [3] and bond analysis using LOBSTER [4]. First, we studied $CrPS_4$ and found an FM ground state with a magnetic moment of 3.0 µB per magnetic atom, consistent with the literature [5]. Detailed analysis of $CrPS_4$'s exchange parameters provided insight into the competition between exchange interaction mechanisms, explaining why it exhibits FM order in the monolayer. We also studied $FePS_4$, $CoPS_4$, $MnPS_4$, and $NiPS_4$. The exchange parameters, combined with structural and COHP analysis, suggest these materials are unstable due to a structure favoring FM ordering. However, the electron distribution in these MPS_4 compounds, except $CrPS_4$, favors AFM coupling.

In conclusion, our study of $CrPS_4$ confirmed the FM ground state and magnetic moment reported in previous literature. We now understand why $CrPS_4$ exhibits FM behavior and envision that this property can be influenced through targeted modifications. Additionally, we provide insights into the instability of other MPS_4 compounds, which can guide experimentalists in modifying these materials to enhance their stability.

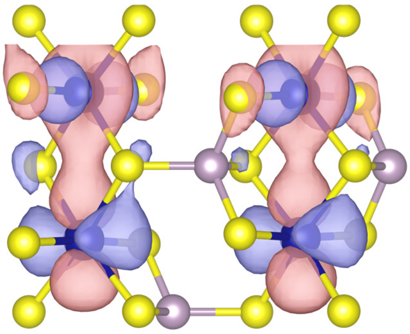

Figure 1. Super-exchange interaction between $CrPS_4$ orbitals (d_{z^2} and d_{xy}).

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Spin State Transitions in FePc Adsorbed on Defected CrI_3

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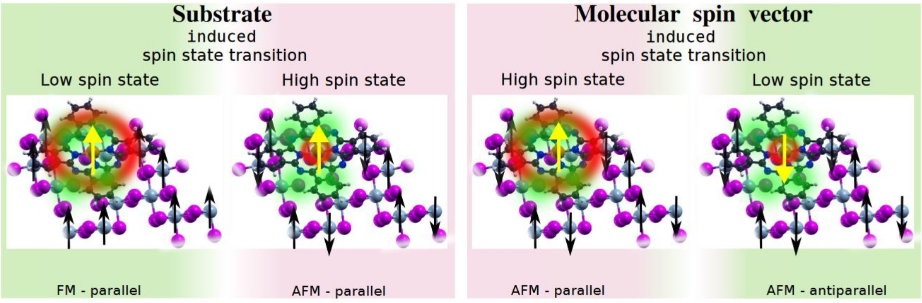
In the realm of molecular spintronics, molecular semiconductors offer a versatile platform enriched with mechanical flexibility, photovoltaic prowess, ferroelectric properties, and magnetic exchange interactions [1-3]. Complementing this, the magnetic behavior of 2D magnet CrI_3 is scrutinized for its layer-dependent characteristics, shedding light on interlayer interactions and magnetic ordering mechanisms [4]. Our investigation delves into the interplay between spin states and iron phthalocyanine (FePc) molecules adsorbed onto defect-functionalized CrI_3 substrates.

We focus on three stable vacancy defects commonly found in CrI_3, created by the removal of '-Cr-', '-I-' and '-CrI_3-' units from the pristine CrI_3 lattice, analyzing by first principle calculations their electronic and magnetic characteristics in both FM and AFM scenarios. FePc demonstrates two stable spin states, a 2 μ_B low spin state and a 4 μ_B high spin state. We present two spin-control mechanisms when FePc adsorbs onto these defect-functionalized substrates: substrate-induced and molecular spin vector-induced control [5]. This research proposes novel effective methods to control the spin states of magnetic metal complexes during adsorption onto magnetic substrates, offering potential applications in molecular electronics and spintronics with 2D materials.



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The impact of organic spacer geometry on electron-phonon coupling in 2D layered Ruddlesden-Popper perovskites

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Two-dimensional layered perovskites, consisting of alternating organic and inorganic layers, have been extensively studied in recent years due to their exceptional optical and electronic properties. One of the most unique properties of these materials is their rather small Young's modulus compared to semiconductor alloys, which makes them prone to phonon-induced lattice deformations. [1] The interaction between electrons and phonons (electron-phonon coupling) can be driven either by deformation potential scattering or piezoelectric interaction with Fröhlich interactions, with longitudinal optical (LO) phonons usually dominant. [2] This effect is attributed to the Coulomb forces between the electrons and the internal electrical field induced by the displacement of oppositely charged atoms caused by the LO modes. By considering the decrease in the bandgap energy related to this phenomenon as well as its increase induced by the thermal expansion of the lattice, the temperature-dependent bandgap can be described with the equation consisting of two opposite parts. [3] Because of the high impact of the optical properties of the materials, the strength of the electron-phonon coupling, and LO phonon energies can be studied through temperature-resolved photoluminescence and absorption spectroscopy. [2,3]

In this work, we studied several two-dimensional Ruddlesden-Popper perovskites with different geometry of the organic spacer. By analyzing the temperature-dependent energy of and shape of the emission, we report the value of the electron-phonon coupling strength as well as the effective energy of LO phonons in respect to the material geometry.

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Electronic and Excitonic Properties of MSi2Z4 Monolayers

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Abstract

MA_2Z_4 monolayers form a new class of hexagonal non-centrosymmetric materials hosting extraordinary spin-valley physics [1]. While only two compounds ($MoSi2N_4$ and $WSi2N_4$) were recently synthesized, theory predicts interesting (opto)electronic properties of a whole new family of such two-dimensional materials [2]. Here, the chemical trends of band gaps and spin-orbit splittings of bands in selected MSi_2Z_4 (M = Mo, W; Z = N, P, As, Sb) compounds are studied from first-principles. Effective Bethe-Salpeter-equation-based calculations reveal high exciton binding energies. The evolution of excitonic energies under an external magnetic field is predicted by providing their effective g-factors and diamagnetic coefficients, which can be directly compared to experimental values. In particular, large positive g-factors are predicted for excitons involving higher conduction bands. In view of these predictions, MSi_2Z_4 monolayers yield a new platform to study excitons and are attractive for optoelectronic devices, also in the form of heterostructures. In addition, a spin-orbit-induced bands inversion is observed in the heaviest studied compound, WSi_2Sb_4, a hallmark of its topological nature.

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Figures

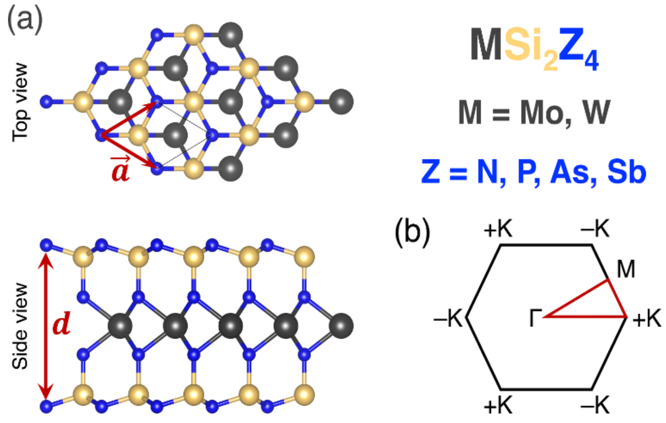

Figure 1: (a) Top and side views of 1L MSi_2Z_4 monolayer generic structure. Hexagonal unit cell is marked together with lattice vector a and the layer thickness d, defined as a distance between the outermost Z atoms. (b) The corresponding hexagonal BZ with the high-symmetry points and a path for band structure calculations (red lines).

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