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UAAT-ICU Workshop: International Taiwan – Czech Event on Research, Innovation, and Education – Prague, Czech Republic, 14–17 July 2025







Vítejte! - Welcome!

Dear Colleagues and Honored Guests,

It is a great pleasure to welcome you to the *UAAT-ICU Workshop: International Taiwan–Czech Event on Research, Innovation, and Education.* This gathering marks a significant moment in the growing scientific collaboration between the Czech Republic and Taiwan - two partners united by a shared commitment to innovation, education, and the advancement of high-tech and next-generation technologies.

Our partnership is built on strong foundations. Taiwan is a global leader in semiconductors and advanced electronics, while Czechia brings deep expertise in materials science, instrumentation, and condensed matter physics. Together, these complementary strengths create a powerful synergy for scientific discovery and technological innovation.

A particularly exciting focus of our collaboration lies in the exploration of van-der-Waals heterojunctions - atomically engineered materials with vast potential for optoelectronics, photonics, and quantum technologies. Projects such as the UAAT initiative demonstrate the impact of joint research and academic exchange, connecting leading institutions like NTNU, NTU, Charles University, the Heyrovský Institute, and the QM4ST consortium.

This workshop is more than a scientific meeting - it is a step forward in building lasting academic alliances, promoting researcher and student mobility, and fostering industry engagement. It reflects our mutual dedication not only to pushing the frontiers of science, but also to training the next generation of innovators.

I extend my warmest wishes for a productive and inspiring workshop. May our conversations here spark new ideas, deepen our cooperation, and contribute to meaningful progress in science and society.

Thank you, and I look forward to the achievements this partnership will bring.

Jana K. Vejpravová Chair of the Symposium









PROGRAM

Monday, July 14 – campus Troja (C126)

12:00 – 13:00 Registration, networking, light refresh	nment

13:00 – 13:15 <u>Welcome and Opening</u> :	Prof. Jana Kalbáčová Vejpravová, Ph.D. & doc. Jiří Pavlů, Ph.D vice-dean for Physics, Charles University
<i>13:15 – 13:30 – <u>Invited</u> (<u><i>I.01</i></u>):</i>	doc. Jan Prokleška, Ph.D., Charles University: Materials Growth & Measurement Laboratory Czech open access research infrastructure
<i>13:30 – 13:55 – <u>Invited (1.02)</u>:</i>	Prof. <u>Ting-Hua Lu</u> , Ph.D., National Taiwan Normal University: <i>Optical Chirality and Exciton-Phonon</i> <i>Coupling in MoS</i> ₂
13:55 – 14:20 – <u>Invited (1.03)</u> :	Prof. <u>Mario Hofmann</u> , Ph.D., National Taiwan University: Unmasking the Intrinsic Spin Dynamics at the Interfaces of 2D materials and Ferromagnets
14:20 – 14:45 – <u>Invited (1.04)</u> :	Prof. <u>Yann-Wen Lan</u> , Ph.D., National Taiwan Normal University: <i>Stacking - and Magnetic Field-</i> <i>induced Polar Order in MoS</i> ₂

14:45 - 15:05 - coffee break, networking

15:05 – 16:30 – lab tour I Material Growth and Measurement Laboratory (MGML)

<u>Free time</u>









<u>Tuesday</u>, July 15 – campus Karlov (F2)

9:30 – 9:55 – <u>Invited (1.05)</u> :	<u>Aleš Melzer</u> , Charles University: Magneto-optical spectroscopy as an effective probe to electronic structure
9:55 - 10:20 - <u>Invited (1.06)</u> :	Prof. <u>Yu-Chiang Chao</u> , Ph.D., National Taiwan Normal University: <i>Optoelectronic Devices based on</i> <i>Chiral Halide Perovskites and Organic</i> <i>Semiconductors</i>

10:20 - 10:40 - <u>coffee break</u>

10:40 – 11:40 – <u>lab tour ^aII (magneto-optical lab, technology lab)</u>

<u>Lunch break 11:40 – 12:40</u>	
12:40 – 13:05 – <u>Invited (I.07)</u> :	Prof. <u>Wen-Chin Lin</u> , Ph.D., National Taiwan Normal University: <i>Modulation of Magnetic Domain and</i> <i>Coercivity in 2D van der Waals Material Fe</i> ₃ <i>Ga</i> ₂ <i>Te</i> ₂
13:05 – 13:30 – <u>Invited (I.08)</u> :	<u>Milan Dopita</u> , Ph.D., Charles University: X-ray Diffraction and Complementary Techniques for the Structural Analysis of Nanostructured and Functional Materials

13:30 - 14:30 - <u>lab tour ^bII (X - ray lab)</u>

<u>Free time</u>









Wednesday, July 16 – Heyrovsky Institute (room 108)

9:30 <u>Welcome</u>	
9:35 – 9:55 – <u>Invited</u> (<i>I.09</i>):	doc. Ing. <u>Kalbáč Martin</u> Ph.D., DSc, J. Heyrovský Institute of Physical Chemistry: <i>UHV exfoliation on</i> <i>the surface of reactive metals</i>
9:55 – 10:15 – <u>Invited (I.10)</u> :	Frank Otakar Ph.D., J. Heyrovský Institute of Physical Chemistry: On the importance of tip- enhanced spectroscopy when characterizing 2D materials
<i>10:15 – 10:35–</i> <u>Invited (<i>I.11</i>)</u> :	Dr. <u>Luka Pirker</u> , J. Heyrovský Institute of Physical Chemistry: <i>The Role of Metallic Substrates in Large-</i> <i>Area Exfoliation of TMDCs</i>
10:35 – 10:55– <u>coffee break</u>	
10:55 – 11:15 – <u>Invited (I.12)</u> :	Ing. <u>Oleksandr Volochanskyi</u> , J. Heyrovský Institute of Physical Chemistry: <i>Graphene-templated Achiral</i> <i>Hybrid Perovskite: Unlocking Circularly Polarized</i> <i>Emission & Sensing</i>
<i>11:15 – 11:40 – <u>Invited (I.13)</u>:</i>	Prof. <u>Ya-Ping Chiu</u> , Ph.D., National Taiwan University: Cross-sectional STM for investigating interface property in heterostructures and future electronics
<i>11:40 – 11:50 – <u>Invited (I.14)</u>:</i>	<u>Li-Sheng Lin</u> , National Taiwan University: Interlayer Coupling in MoS_2 on $Bi(110)$ and $Bi(111)$: A First- Principles Investigation
<i>11:50 – 12:00 – <u>Invited (I.15)</u>:</i>	Yan-Ruei Lin, National Taiwan University: Atomically Resolved Interlayer Coupling in MoS ₂ on Bi(110) and Bi(111)

<u>12:00 – 13:30 Lunch break</u>

13:30 – 15:00 – lab tour III Dept. of low-dimensional systems, Dept. of electrochemical materials
<u>Free time</u>
18:00 – 22:00 – dinner <u>Pivovar Ládví Cobolis</u>, Burešova 1661/2, 182 00 Praha 8-Kobylisy (metro Ládví)









Thursday, July 17 – campus Troja (C126)

<i>10:00 – 10:20 – <u>Invited (I.16)</u>:</i>	Daowei Wang, Ph.D., Charles University: <i>Guided</i> exchange-dipole spin wave in monolayer CrSBr
10:20 – 10:40 – Invited (I.17):	Vaibhav Varade , Ph.D., Charles University: Isotope Engineering in Two-Dimensional Transition Metal Dichalcogenides and Their Hetero-bilayers
<i>10:40 – 11:00 – <u>Invited (I.18)</u>:</i>	Rahul Kesarwani, Ph.D., Charles University: <i>Giant</i> <i>Polarisation Ratio in Chiral Photoluminescence from</i> <i>MoS</i> ₂ <i>Nanorolligami via Centre-to-Edge Rolling</i>

11:00 - 12:20 - lab tour IX (surface science group), round table discussion and refreshments

<u>Closing</u> ~ 12:20

~12:30 – 13:00 – *closing lunch*

13:30 - Guided tour - Prague Castle, Old Town









I.01

Materials Growth & Measurement Laboratory Czech open access research infrastructure

Jan Prokleška

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ABSTRACT

In this contribution, the Materials Growth & Measurement Laboratory (MGML https://mgml.eu/) will be introduced as a unique research infrastructure dedicated to the comprehensive experimental study of materials under precisely controlled external conditions. The core mission of MGML is to support the international scientific community by providing open access to a broad range of advanced instrumentation for measurements of physical properties across wide temperature ranges, magnetic and electric fields, and under hydrostatic or uniaxial pressure. Alongside its measurement capabilities, MGML offers facilities for the controlled growth and characterization of high-quality single crystals and polycrystalline samples, available also to users who do not have access to well-characterized specimens of their own. Selected scientific results obtained within MGML will be presented to illustrate the breadth and versatility of the infrastructure and its potential to enable high-impact research across condensed matter physics, materials science, and related fields.









I.02

Optical Chirality and Exciton-Phonon Coupling in MoS2

<u>**Ting-Hua Lu**</u>, Yu-Chen Chang, Yu-Chiao Chan and Yann-Wen Lan Department of Physics, No.88 Sec. 4 Tingchou Rd, Taipei, Taiwan

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ABSTRACT

Molybdenum disulfide (MoS_2) , a prototypical two-dimensional transition metal dichalcogenide, exhibits excitation-energy-dependent photoluminescence and Raman responses that are highly sensitive to material conditions. In this talk, I will present our investigation of phonon symmetry and exciton-phonon interactions in MoS_2 under double- resonance Raman conditions using optically spin-polarized excitation and detection. Temperature-dependent Raman and photoluminescence spectroscopy were performed under polarized excitations at 532 nm and 633 nm. Our experimental and numerical results reveal notable symmetry changes in the degenerate in-plane phonon modes, driven by variations in exciton-phonon coupling strength via the Fröhlich interaction. Both monolayer and bilayer MoS_2 exhibit phonon symmetry modifications correlated with exciton spin-valley polarization under resonance conditions. These findings underscore the significance of Fröhlich-type interactions in shaping Raman-active phonon behavior and provide new insights into spin-dependent exciton dynamics in two-dimensional semiconductors.

Keywords: transition metal dichalcogenides; electron-phonon interactions; double- resonance Raman.

References:

[1] Yu-Chen Chang, Yu-Chiao Chan, Bipul Das, Jiao-Fang Syue, Hsiang-Chi Hu, Yann-Wen Lan*, and Ting-Hua Lu*, "Distinctive characteristics of exciton-phonon interactions in optically driven MoS2", 2024, Phys. Rev. Materials 8, 074003 (2024)









I.03

Unmasking the Intrinsic Spin Dynamics at the Interfaces of 2D materials and Ferromagnets

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ABSTRACT

The integration of two-dimensional (2D) materials into spintronic devices has long promised revolutionary improvements in performance and energy efficiency, yet progress has been hampered by interface contamination, oxidation-induced magnetic pinning, and compromised transmission at the 2D/ferromagnetic (FM) junction. In our work, we introduce an advanced, single-step deposition process that simultaneously deposits asymmetric FM contacts onto atomically thin barriers such as graphene and molybdenum disulfide (MoS₂), thereby achieving pristine, ultra-clean interfaces.

Leveraging this novel fabrication method mediates oxidation and contamination effects and reveals the intrinsic response of the 2D/FM junction. The resulting devices demonstrate exceptional magnetoresistance and significantly reduced coercivity, directly reflecting the inherent properties of the 2D interface. We observe a novel metallization effect between MoS2 and its contacts. The use of multilayer MoS₂ not only suppresses metallization effects but also restores semiconducting behavior, facilitating robust spin-filtering and yielding record-negative magnetoresistance values. Our advances underscore the critical importance of precise interface engineering in optimizing spin injection and magnetic anisotropy for the development of next-generation, 2D spintronic devices.

Keywords: 2D materials; spintronics; magnetism; carrier transport;

References:

[1] Ting-Chun Huang, Wen-Hua Wu, Meng-Ting Wu, Chiashain Chuang, Chi-Feng Pai, Ya-Ping Hsieh, and Mario Hofmann, ACS Materials Letters 2024 6 (1), 94-99, DOI: 10.1021/acsmaterialslett.3c01194









I.04

Stacking - and Magnetic Field-induced Polar Order in MoS₂

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ABSTRACT

Recent breakthroughs in ferroelectric memory and valleytronic devices have highlighted the unique functionalities of rhombohedral-stacked (3R) bilayer molybdenum disulfide (MoS₂) and monolayer transition metal dichalcogenides (ML-TMDs). We report on the realization of a ferroelectric memory transistor based on 3R-stacked bilayer MoS₂, where asymmetrical stacking results in spontaneous out-of-plane electric polarization [1]. This ferroelectric property grants non-volatile memory characteristics, making it suitable for low-power, high-density memory applications. Additionally, monolayer MoS₂ with broken inversion symmetry and strong spin-orbit coupling exhibits spin-valley lock-in effects, allowing magnetic fields to lift valley degeneracy and potentially induce real-space structural transformations. The resulting broken symmetry-induced polarization in ML-MoS₂ demonstrates ferroelectric hysteresis, thus adding ML-MoS₂ to the family of monolayer materials with out-of-plane polar order-induced ferroelectricity [2]. These findings suggest promising applications for ML-MoS₂ in cryogenic ultracompact non-volatile memories, memtransistors, and highly sensitive magnetic field sensors, advancing the field of 2D material-based electronic and spintronic devices.



Keywords: valleytronic devices; molybdenum disulfide (MoS₂);

Reference:

- Yang, T.H., Lan, Y.W et al. Ferroelectric transistors based on shear-transformation-mediated rhombohedral-stacked molybdenum disulfide. Nat Electron 7, 29–38 (2024). https://doi.org/10.1038/s41928-023-01073-0
- [2] D. Hao, W.-H. Chang, Y.-C. Chang, W.-T. Liu, S.-Z. Ho, C.-H. Lu, T. H. Yang, N. Kawakami, Y.-C. Chen, M.-H. Liu, C.-L. Lin, T.-H. Lu, Y.-W. Lan, N.-C. Yeh, Magnetic Field-Induced Polar Order in Monolayer Molybdenum Disulfide Transistors. *Adv. Mater.* 2024, 2411393. <u>https://doi.org/10.1002/adma.202411393</u>









I.05

Magneto-optical spectroscopy as a probe to electronic structure and magnetism of materials and nanostructures

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ABSTRACT:

Magneto-optical effects play an important role in both research and application fields. Magnetooptical experiments are widely used as non-destructive, depth sensitive and extremely precise tools to explore basic and novel physical phenomena and properties of magnetic materials. Magnetic field dependent magneto-optical measurements under different field orientations can provide a useful insight into the magnetic anisotropy of studied materials even for very small magnetizations. On the other hand, one can use spectrally dependent measurements in combination with ab-initio calculations to analyze electronic transitions across the band structure to map particular electronic states with large splitting. Moreover, a combination of the field and spectrally dependent magneto-optical measurements, which gives energy dependent hysteresis loops, can provide useful insight into the magnetism of various sublattices in multi-sublattice magnetic systems, interface phenomena or surface magnetism. The talk will provide an overview the recent magneto-optical research in the field of La_{2/3}Sr_{1/3}MnO₃ and SrRuO₃ thin films for efficient control of the electron spin.









I.06

Optoelectronic Devices based on Chiral Halide Perovskites and Organic Semiconductors

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ABSTRACT

Halide perovskites are one of the most promising materials for photovoltaic and light-emitting devices. Chiral 2D halide perovskites can be obtained by introducing chiral organic halides such as R- and S-methylbenzylammonium halide and R- and S-1-(2-naphthyl)ethylammonium halide. Similarly, introducing chiral dopants can produce organic semiconductors with chirality. These semiconducting materials will exhibit chiroptical properties. Circularly polarised light-emitting diodes based on these materials will also be demonstrated.[1-3]

Keywords: Chirality; Perovskites; Organic semiconductors

References:

ACS Appl. Mater. Interfaces 14, 54090 (2022)
 Mater. Horiz. 12, 1863 (2025)
 Small Sci. 2500034 (2025)









I.07

Modulation of Magnetic Domain and Coercivity in 2D van der Waals Material Fe₃Ga₂Te₂

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ABSTRACT

Microscopic spin textures in two-dimensional (2D) van der Waals (vdW) ferromagnets are promising for next-generation spintronic devices, offering high data density and low energy consumption. Among these materials, Fe₃GaTe₂ (FGT) is notable for its high Curie temperature (above room temperature) and stable perpendicular magnetic anisotropy (PMA). Precise control of magnetic domains in FGT is essential for advancing practical spintronic applications.

In this study, we investigate the evolution of magnetic domain structures in both thin and thick FGT flakes during field cooling (FC). A transition from stripe to bubble and complex domain configurations is observed, with domain size increasing as the FC magnetic field strength increases. Bubble and complex domains remain stable above 2000 Oe, indicating robust spin textures. The application of external magnetic fields leads to further domain enlargement, and hexagonal ordering of magnetic bubbles emerges through field-induced splitting and reshaping processes. Domain elimination and merging phenomena are also demonstrated.

Micromagnetic simulations reproduce the experimental observations and reveal size- and timedependent domain dynamics. In addition, local pressure applied via contact-mode atomic force microscopy (AFM) significantly reduces the coercivity of FGT flakes. The relationship between coercivity and relevant parameters is systematically analyzed.

These findings provide valuable insights into the tunable magnetic properties of FGT and underscore its potential for domain engineering and spin transport control in spintronic applications.

Keywords: Magnetism; 2D Material; Magnetic Domain; Magnetic Coercivity;

Reference:

Chak-Ming Liu, Yi-Jia Liu, Po-Chun Chang, Po-Wei Chen, Masahiro Haze, Ming-Hsien Hsu, Neleena Nair Gopakumar, Yishui Zhou, Yung Hsiang Tung, Sabreen Hammouda, Chao-Hung Du, Yukio Hasegawa, Yixi Su, Hsiang-Chih Chiu, Wen-Chin Lin *Appl. Surf. Sci. Adv. 26, 100718 (2025).*









I.08

Instrumentation and experimental facilities of the X-ray laboratory at the DCMP, MFF UK

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ABSTRACT

In last few years the x-ray laboratory at the Department of Condensed Matter Physics, leading laboratory on the field of x-ray scattering in the Czech Republic and very well distinguished worldwide, underwent significant instrumental upgrade. Several modern – top class laboratory instruments substantially broadening the instrumental possibilities and available scattering techniques of the laboratory were commissioned. Namely i) the general purpose x-ray diffractometer equipped with a high flux rotation anode x-ray source and goniometer allowing both, coplanar and non-coplanar (inplane) diffraction; ii) high energy x-ray diffractometer equipped with unique x-ray optical elements, operating with various x-ray energies (6.9 - 22 keV); and iii) apparatus dedicated to a small angle x-ray scattering (SAXS) and small angle x-ray scattering in non-coplanar geometry (GISAXS) measurements. All machines are equipped with modern 2D hybrid pixel, single photon counting, low noise, detectors.

This unique combination of x-ray diffractometers offers measurements covering a wide range of reciprocal space between q of 0.003 to 21 1/Å (q is a magnitude of reciprocal space vector), which allows the fundamental studies of materials properties in ranges from 0.03 up to 200 nm, in real space. The equipment represents a unique collection of instruments allowing nearly any type of laboratory accessible x-ray scattering experiment - measurements of single crystals, polycrystalline bulk and powder materials, nanocrystalline samples, thin films, multilayers and epitaxial layers.

The instruments can operate with various x-ray wavelengths (Co, Cu, Mo and Ag), and in different geometries: Bragg-Brentano geometry, medium resolution parallel beam setting, high resolution geometry, with monochromatic K α 1 radiation and in coplanar and non-coplanar (in-plane) mode. Various sample environments, low and high temperature chambers, deformation (tensile and compression) stage, reaction chamber are available for individual diffractometers. Methodologically the laboratory offers the structure solution and refinement, qualitative and quantitative phase analysis, the real structure of material studies: preferred orientation of crystallites – texture measurements, residual stress measurements, reflectivity measurements, rocking curve measurements, reciprocal space mapping, pair distribution function – total scattering measurements, small angle x-ray scattering and grazing-incidence small angle x-ray scattering.

In the lecture the experimental abilities of our x-ray laboratory together with examples of individual applications (with the focus to a special, challenging, or non-commonly used techniques) in materials research will be shown and discussed in details.









I.09

UHV exfoliation on the surface of reactive metals

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ABSTRACT

2D materials are extremally sensitive to their environment. This is because they do not have a bulk component and thus literally all atoms can interact with species adhering to the surface of the 2D material. In ambient conditions the surface gets immediately covered by impurities. In order to preserve a clean surface, we propose a method for exfoliation of the 2D materials in ultra-high vacuum conditions. In this work, we utilize fresh titanium layer as a substrate for exfoliating MoS2 under UHV. Exfoliation of MoS2 on Ti resulted in a centimetre-scale layer, similar in size to the parent bulk crystal. However, Raman and XPS analyses reveal that the strong reactivity of the fresh Ti surface decomposes the first MoS2 layer, leaving it in a predominantly metallic Mo state.

Keywords: UHV exfoliation, spectroscopy, 2D materials









I.10

On the importance of tip-enhanced spectroscopy when characterizing 2D materials

Otakar Frank¹,* Luka Pirker¹, Alvaro Rodriguez¹, Matěj Velický¹

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*Corresponding Author E-mail: <u>Otakar.frank@jh-inst.cas.cz</u>

ABSTRACT

Common spectroscopic investigation of two-dimensional materials and their van der Waals (vdW) heterostructures mostly relies either on diffraction-limited microRaman or photoluminescence (PL). However, these methods do not properly capture local variations caused by, e.g., nanometre-sized heterogeneities stemming from contamination trapped between the layers or complex strain and charge patterns formed by strong out-of-plane interactions.

Tip-enhanced spectroscopy methods enable access to information on the local lattice deformation and also on the interaction between the individual layers composing the heterostructure. What may appear as peak splitting in micro-Raman or PL spectra of transition metal dichalcogenides (TMDC) on metal substrates or of vdW heterobilayers can, in fact, often come from mixing up signals from various regions within the laser spot, including new or discretely shifted peaks. In other cases, however, peak splitting can indicate lifting the degeneracy of the phonon, due to, for example, uniaxial deformation. Nanospectroscopic fingerprints of variously interacting vdW layers will be discussed, including TMDCs on metals [1-3] and TMDC heterobilayers [4-6].

Keywords: tip-enhanced spectroscopy; Raman, photoluminescence, 2D materials.

References (Times new roman, font size 10):

- [1] Velicky et al. J. Phys. Chem. Lett. 11, 6112 (2020)
- [2] Velicky et al. Adv. Mater. Interfaces 7, 2001324 (2020)
- [3] Rodriguez et al. Phys. Rev. B 105, 195413 (2022)
- [4] Rodriguez et al. 2D Mater. 8, 025028 (2021)
- [5] Rodriguez et al. J. Phys. Chem. Lett. 13, 5854 (2022)
- [6] Rodriguez et al., ACS Nano 17, 7787 (2023)









The Role of Metallic Substrates in Large-Area Exfoliation of TMDCs

Luka Pirker^{1,*}, Michaela Hanušová^{1,2}, Václav Valeš³, Martin Vondráček³, Jan Honolka³, Otakar Frank¹ and Matěj Velický¹

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ABSTRACT

Gold-assisted exfoliation has proven to be an effective method for selectively obtaining large-area monolayers of transition metal dichalcogenides (TMDCs), though its underlying mechanism remains a topic of debate [1,2]. While other metals can also facilitate exfoliation, their practical application is often hindered by surface oxidation [3].

In this study, we systematically examine six MoS_2 /metal heterostructures, prepared via direct mechanical exfoliation onto metallic surfaces under controlled atmospheric conditions (Fig. 1a-f). Our analyses, conducted using ultraviolet photoelectron spectroscopy, X-ray photoelectron spectroscopy, and Raman spectroscopy (Fig. 1g), reveal substantial differences in interfacial interactions depending on the chosen metal. Density functional theory calculations further support these variations. These findings highlight the influence of metal substrates on the electronic structure and vibrational properties of MoS_2 and offer key insights into the mechanisms driving metal-assisted exfoliation.



Figure 1. (a-f) Optical images of large-area MoS_2 monolayers exfoliated on Cu, Ag, Au, Co, Ni, and Pd. (g) Raman spectra of MoS_2 monolayers exfoliated on different metals.

Keywords: MoS₂; Metal assisted exfoliation; Raman spectroscopy; Photoemission spectroscopy.

References:

- [1] Velický, Matej, et al., ACS nano, 12(10), 10463-10472, (2018)
- [2] Ziewer, Jakob, et al., Advanced Materials, 2419184, (2025)
- [3] Velický, Matěj, et al., Advanced Materials Interfaces, 7(23), 2001324, (2020)









I.12

Graphene-templated Achiral Hybrid Perovskite: Unlocking Circularly Polarized Emission & Sensing

<u>Oleksandr Volochanskyi^{1,2}</u>, Golam Haider¹*, Essa A. Alharbi^{3,4}, George Kakavelakis^{4,5}, Martin Mergl¹, Mukesh Kumar Thakur¹, Anurag Krishna⁴, Michael Graetzel⁴, Martin Kalbáč¹*

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ABSTRACT

The spin degree of freedom and its manipulation has become a hot research topic across the material sciences, with the goal of developing next-generation spintronic and photonic devices. In this work, we demonstrate that single-layer graphene can template the growth of achiral α -FAPbI₃ perovskite into a "chiral" composite heterostructure exhibiting Rashba-type band splitting at ambient conditions. During the perovskite deposition, interactions at the graphene interface promote structural distortions, leading to local inversion symmetry breaking at the perovskite/graphene heterojunction and enabling efficient spin-charge conversion under circularly polarized light.

We achieve a circularly polarized photoluminescence anisotropy factor (g_{CPL}) of ~0.35 and a spinpolarized photocurrent anisotropy factor (g_{ph}) up to ~0.51, accompanied by a high photoresponsivity of ~10⁵ A/W at low illumination fluence. Importantly, reducing the perovskite thickness enhances the g_{ph} factor, underscoring the interfacial origin of the spin polarization. These results demonstrate how graphene-mediated growth can be leveraged to engineer spin-sensitive optoelectronic responses in halide perovskites, offering a new route toward compact, polarization-sensitive optoelectronic devices.

Keywords: Rashba splitting; Graphene; Perovskite; Photodetector.









I.13

Cross-sectional STM for investigating interface property in heterostructures and future electronics

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ABSTRACT

Interface science has recently received significant attention due to the development of state-ofthe-art materials and devices that provide powerful ways to create and manipulate charge, spin, orbital, and lattice degrees of freedom at interfaces. Motivated by the fact that nanoscale interface science is critical for device applications, this talk will focus on sharing the measurement capabilities of mapping the interfacial properties of heterostructured structures using cross-sectional scanning tunneling microscopy (XSTM) and elucidating the mechanisms inherent in these materials and devices.

In my lab, the establishment of the XSTM technique has provided a measurement tool for probing the electronic structure and band alignment of interfaces in cutting-edge heterostructured materials. Recently, the platform has been combined gate-, source- and drain- tunable biasing and will be used to explore the electronic structure of cutting-edge device interfaces. This will be a potential demonstration of characterization capabilities and provide critical insights into the exploration and innovation of future electronic devices.

Keywords: scanning tunneling microscopy; interface; heterostructures; future electronics.

Reference:

[1]: Chun-Chih Hsu, Bo-Chao Huang, Michael Schnedler, Ming-Yu Lai, Yuh-Lin Wang, Rafal E. Dunin-Borkowski, Chia-Seng Chang, Ting-Kuo Lee, Philipp Ebert, Ya-Ping Chiu, *Nature Communications* volume 12, 3893 (2021).

[2] Pei-Rui Luo, Hung-Chang Hsu, Hao-Yu Chen, Xiang-Yu Xie, Chia-Nung Kuo, Chin-Shan Lue*, Ya-Ping Chiu*. Direct Evidence of Coupling between Charge Density Wave and Kondo Lattice in van der Waals Ferromagnet Fe5GeTe2. *Nature Communications* 16, 5080 (2025).









I.14

Interlayer Coupling in MoS₂ on Bi(110) and Bi(111): A First-Principles Investigation

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ABSTRACT

Ultra-thin two-dimensional (2D) semiconductors are considered promising candidates for nextgeneration electronic devices due to their atomically flat surfaces and tunable van der Waals (vdW) interactions. For most metal/semiconductor contacts, metal-induced gap states (MIGS) lead to increased contact resistance. However, recent studies have shown that semimetallic bismuth (Bi) forms nearly Ohmic contacts with transition metal dichalcogenides (TMDs)^{1,2}. The atomistic origin of this favorable coupling, however, remains unelucidated. In this work, we employ first-principles density functional theory (DFT) calculations to investigate the electronic structure of molybdenum disulfide (MoS₂) in contact with Bi substrates at different crystallographic orientations. Our results reveal distinct interlayer coupling and electronic behaviors depending on the relative orientation between MoS2 and the underlying Bi(110) and Bi (111) surfaces. This study provides theoretical insights into how crystallographic orientation and interfacial coupling between TMDs and semimetals influence the electronic properties of TMDs, thereby offering valuable guidance for the design and optimization of future TMD-based electronic devices.

Keywords: transition metal dichalcogenides; molybdenum disulfide; density functional theory. Bismuth (110); interlayer coupling

References:

- 1. Shen, P.-C. et al. Ultralow contact resistance between semimetal and monolayer semiconductors. Nature 593, 211-217 (2021).
- Chen, Y.-F. et al. Direct Visualization of Metal-Induced Gap State Distribution and Valley Band Evolution at Metal Versus Semimetal MoS2 Interfaces. ACS Nano, 19, 19408–19416 (2025)









I.15

Atomically Resolved Interlayer Coupling in MoS2 on Bi(110) and Bi(111)

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ABSTRACT

Ultra-thin two-dimensional (2D) semiconductors are considered promising candidates for nextgeneration electronic devices due to their atomically flat surfaces and tunable van der Waals (vdW) interactions. For most metal/semiconductor contacts, metal-induced gap states (MIGS) lead to increased contact resistance. However, recent studies have shown that semimetallic bismuth (Bi) forms nearly Ohmic contacts with transition metal dichalcogenides (TMDs)^{1,2}. The atomistic origin of this favorable coupling, however, remains unelucidated. In this work, we employ first-principles density functional theory (DFT) calculations to investigate the electronic structure of molybdenum disulfide (MoS₂) in contact with Bi substrates at different crystallographic orientations. Our results reveal distinct interlayer coupling and electronic behaviors depending on the relative orientation between MoS2 and the underlying Bi(110) and Bi (111) surfaces. This study provides theoretical insights into how crystallographic orientation and interfacial coupling between TMDs and semimetals influence the electronic properties of TMDs, thereby offering valuable guidance for the design and optimization of future TMD-based electronic devices.

Keywords: transition metal dichalcogenides; molybdenum disulfide; density functional theory. Bismuth (110); interlayer coupling

References:

- 3. Shen, P.-C. et al. Ultralow contact resistance between semimetal and monolayer semiconductors. Nature 593, 211-217 (2021).
- Chen, Y.-F. et al. Direct Visualization of Metal-Induced Gap State Distribution and Valley Band Evolution at Metal Versus Semimetal MoS2 Interfaces. ACS Nano, 19, 19408–19416 (2025)









I.16

Guided exchange-dipole spin wave in monolayer CrSBr

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ABSTRACT

CrSBr is an air-stable van der Waals antiferromagnet with high Néel temperature, which can have potential application in magnonic devices that use spin wave to transmit information. For this purpose, we investigated the spin-wave spectrum of spin-wave wave guides based on a monolayer of CrSBr, which is the building block of bulk CrSBr, by considering the various magnetic interactions present in CrSBr, including the ferromagnetic exchange interaction, the triaxial anisotropy energy, the Zeeman interaction, and the magnetic dipolar interaction. In contrast to its short-range counterparts, the long-range dipolar field acts statically as a confining potential for the exchange-dipolar spin wave under investigation, while the dynamic dipolar interaction couples the spin and orbital motion of a magnon, thus giving rise to magnonic doublets (cf. Fig. 1) with definite parity under space inversion. Numerical calculation tallies well with results obtained by micromagnetic simulation. Our study on the spin-wave eigenmode for a monolayer of CrSBr sheds light on the nature of exchange-dipole spin wave in a thin ferromagnetic slab; we confirm particularly that there is no topological protection for the Damon-Eshbach mode. Moreover, a thorough knowledge on the spin-wave eigenmode in monolayer CrSBr itself represents a step forward to understanding the more complicated antiferromagnetic resonance in bulk CrSBr.



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Fig. 1. Theoretically calculated (circles) and OOMMF simulated dispersion relations for a monolayer of CrSBr with magnetic field B = 0.7 T applied perpendicular to the CrSBr plane. The dimension of the monolayer is 16384 $nm \times 256 nm \times 1 nm$.

Keywords: CrSBr; spin wave; dipolar interaction.









I.17

Isotope Engineering in Two-Dimensional Transition Metal Dichalcogenides and Their Hetero-bilayers

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ABSTRACT

In this presentation, I will discuss our recent advances in tuning the optoelectronic properties of two-dimensional (2D) transition metal dichalcogenides (TMDCs) through sulfur isotope engineering. By introducing heavier sulfur isotopes during chemical vapor deposition (CVD) growth, we achieved systematic control over lattice phonon energies, which in turn significantly modified both transient and steady-state photoluminescence responses. Isotopically pure monolayers of MoS₂ showed enhanced emission efficiency and more intrinsic excitonic behavior compared to mixed-isotope samples, with temperature-dependent exciton shifts well captured by Varshni's equation.[1]

I will also present our work on constructing a double-layer MoS_2 heterostructure (hetero-bilayer) composed of adjacent monolayers enriched with different sulfur isotopes (${}^{34}S/{}^{32}S$) fabricated via 2-steps CVD.[2] Strong interlayer coupling in this system was confirmed by low-frequency Raman modes, and photoluminescence measurements revealed dominant emission from the ${}^{32}S$ layer, alongside suppressed intralayer excitons and faster exciton lifetimes.

Finally, I will very briefly summarize our results on valley emission and up-conversion phenomena in isotopically engineered monolayer WS_2 under resonant excitation.[3] These results highlight how isotope engineering can be a powerful tool to tailor phonon-exciton interactions and exciton dynamics at the nuclear level, without requiring chemical modification.

Keywords: Isotope engineering; TMDCs; Raman spectroscopy; Exciton dynamics

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[1] Varade et. al., 2D Mater. 10, 025024 (2023)

[2] Varade et. al., Nanoscale Adv. 7, 1276-1286 (2025)

[3] Kesarwani et. al., 2D Mater. 12 (2), 025029. (2025)

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I.18

Giant Polarisation Ratio in Chiral Photoluminescence from MoS₂ Nanorolligami via Centre-to-Edge Rolling

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ABSTRACT

We introduced mechanical strain to systematically roll monolayer (1-L) MoS₂ into nanostructures with diameters ranging from 100 – 200 nm. The rolled MoS₂ regions exhibit unique anisotropic optical behaviour compared to the flat regions (thickness ≤ 1 nm), as analysed through polarisation-resolved photoluminescence (PL) and Raman spectroscopy. Raman spectroscopy revealed that the E_{2g}/A_{1g} intensity ratio under circular polarisation was approximately 0.25 in the rolled regions, whereas it approached zero in the flat region. These findings highlight pronounced optical anisotropy and symmetry-breaking in rolled MoS₂, distinguishing it from the isotropic flat regions. Additionally, angular-dependent PL measurements demonstrated a strongly enhanced linear polarisation ratio (LPR) of 28% and circular polarisation ratio (CPR) of 37% in the rolled regions, indicating strong optical anisotropy. In contrast, the flat MoS₂ regions exhibited isotropic behaviour, with LPR and CPR values typically around 8%.

Our results demonstrate that rolling-induced localised deformation profoundly modifies exciton polarisation behaviour in MoS_2 . Enabling precise light filtering and nanoscale manipulation via nanoscrolling of the two-dimensional materials, our work lays the foundation for next-generation optoelectronic devices with tailored optical responses and enhanced functionality.

project Acknowledgements: The **"MSCA Fellowships** CZ UK3" (reg. n. CZ.02.01.01/00/22_010/0008220) is supported by the Programme Johannes Amos Comenius and **OM4ST** Quantum materials for applications sustainable technologies in CZ.02.01.01/00/22_008/0004572.









Campus Troja, Faculty of mathematics and physics, Charles University, Cryogenics

Laboratory "C" (room C126) V Holešovičkách 747/2, 180 00 Praha 8

How to get there:

From the metro station Nádraží Holešovice line C (red) go two stops by bus 201 to Kuchyňka



Campus Karlov Faculty of Mathematics and Physics Ke Karlovu 5 (*room F2*) *Ke Karlovu 2026/5, 121 16 Praha 2*

Ke Karlovu 2020/3, 121

How to get there:

You can walk from the metro station *I.P. Pavlova* line C (red) to *Faculty of Mathematics and Physics Ke Karlovu 5*, *F*^{*}, or you can take bus *148* one stop *Dětská nemocnice Karlov*











J. Heyrovský Institute of Physical Chemistry (room 108)

Dolejskova 2155/3, Libeň, 182 00 Praha 8

How to get there:

The Heyrovský Institute is only a 10 - minute walk from the metro station *Ládví* line C (red).



Pivovar Ládví Cobolis

Burešova 1661/2, 182 00 Praha 8-Kobylisy **How to get there:** The *Pivovar Ládví Cobolis* is only a 1 - minute walk from the *Ládví* metro station











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Orientační plán metra

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