

Two-Dimensional Materials

Book of Abstracts

56th Heyrovský Discussions

June 8-12, 2025, Třešť, Czech Republic



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Prof. Jaroslav Heyrovský (20. 12. 1890 – 27. 3. 1967)

Academician Jaroslav Heyrovský is widely regarded as the founder of polarography (1922) —a groundbreaking analytical method for the rapid and precise determination of metals and their concentrations in solution.

In 1924, together with his Japanese apprentice Masuzo Shikata, Heyrovský designed and built the first automatic instrument for this technique, which he named the polarograph.

Following World War II, polarography saw widespread adoption across science, medicine, and various industries, marking a period of significant expansion for the method. In 1950, Heyrovský established the Institute of Polarography, which became part of the Academy of Sciences in Prague.

Jaroslav Heyrovský remains the only Czech scientist to have received the Nobel Prize in Chemistry (1959), in recognition "for his discovery and development of the polarographic methods of analysis".

The tradition of the Heyrovský Discussions began in 1967 and has continued ever since under the auspices of the Czech Academy of Sciences. Originally held at the Liblice Castle, the Discussions later moved to the Bechyně Castle and, more recently, to the Renaissance Chateau in Třešť. Nestled in the scenic and historically rich landscape of southeastern Bohemia, Třešť offers a tranquil and inspiring setting for scientific exchange.



Sunday, June 8

14:00	Registration in the entrance hall of the J. Heyrovský Institute
15:00	Departure of a charter bus from the J. Heyrovský Institute (Dolejšková 3, Prague 8)
17:00	Arrival at the Chateau Třešť, registration
18:30	Welcome buffet

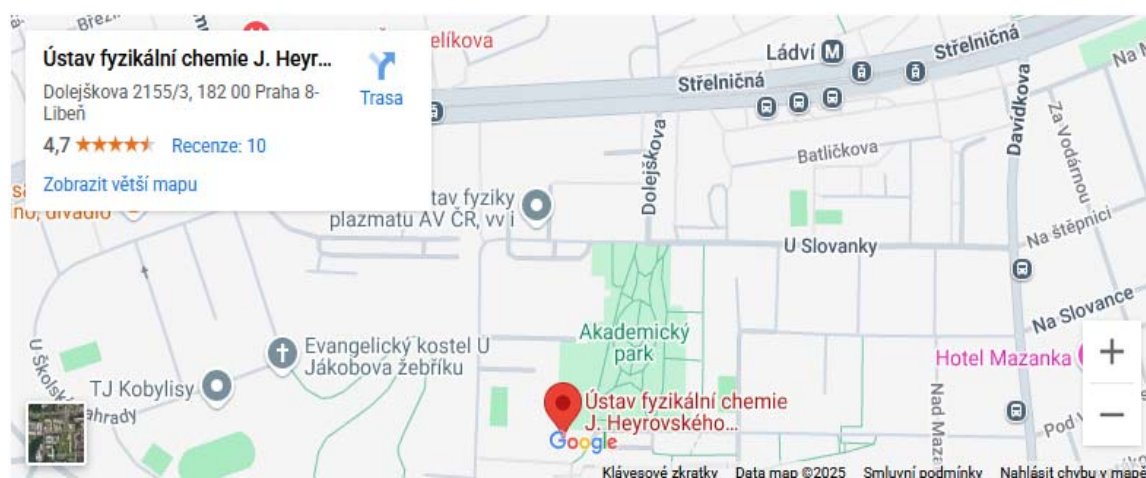
How to reach the J. Heyrovský Institute

By metro: take line C to the station Ládví and walk for about 4 min

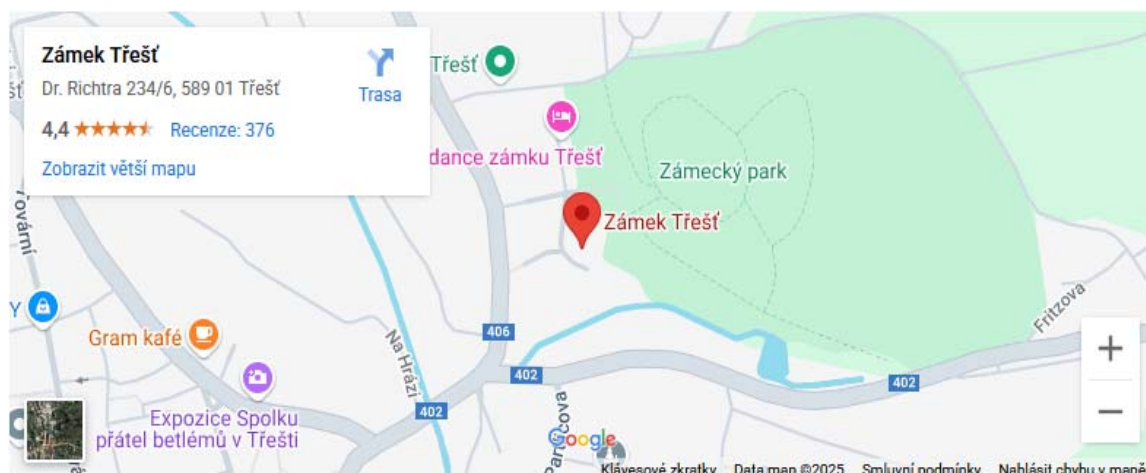
By tram: No. 10 to the stop Ládví

By car: via Davidkova street and Pod vodárenskou věží street to the Institute

The Institute will be open on Sunday from 10:00 for possible luggage deposit.



The Renaissance Chateau Třešť is located in the small town of Třešť, in southeastern Bohemia, about 15 km south of Jihlava (which is situated on the highway D1 Prague-Brno, approx. 120 km from Prague), in an attractive, peaceful locality rich in historical monuments and of beautiful natural scenery.



Monday, June 9

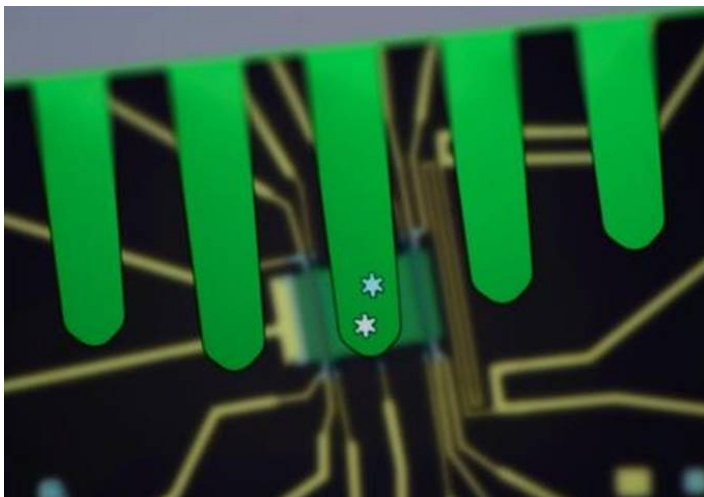
7:00-9:00	Breakfast		
9:00	Morning session:		
	Opening of the Discussions		
<i>Time</i>	<i>Chair</i>	<i>Speaker</i>	<i>Title of presentation</i>
9:05-9:45	M. Velický	R. Gorbachev	Ultraclean van der Waals Heterostructures
9:45-10:05		F. Huang	Mechanism of Gold-Assisted Exfoliation
10:05-10:25		S. Debnath	Investigating MBE growth and characterization of MoS ₂ on Au(788) using ARPES and Raman Spectroscopy
10:25	Coffee break		
<i>Time</i>	<i>Chair</i>	<i>Speaker</i>	<i>Title of presentation</i>
10:55-11:35	K. Bediako	J. Sambur	Band gap renormalization effects on electrochemical currents at 2D semiconductor/electrolyte interfaces
11:35-11:55		M. Jindra	In-situ Raman (Spectro)Electrochemical Study of Intact and Defective Monolayer Graphene
11:55-12:15		M. Velický	Spatial Dynamics of the Fermi Level in Electrolyte-Gated Graphene
12:15	Lunch		
14:30	Afternoon session:		
<i>Time</i>	<i>Chair</i>	<i>Speaker</i>	<i>Title of presentation</i>
14:30-14:50	R. Gorbachev	S. Sahu	Exploring Resonance Raman Scattering and Stimulated Raman Scattering Effects in CrSBr
14:50-15:10		V. Valeš	Stability of transition metal thio(seleno)phosphate monolayers on gold substrates
15:10-15:30		T. Verhagen	Sliding ferroelectricity in misfit layer compound (PbS) _{1.11} VS ₂
15:30-15:50		P. Barath	Get to know Metrohm
15:50	Coffee break + Poster session I		
<i>Time</i>	<i>Chair</i>	<i>Speaker</i>	<i>Title of presentation</i>
17:20-18:00	M. Kalbáč	R. Dryfe	Controlling Wetting on Carbon Surfaces
18:30	Buffet dinner		

Ultraclean van der Waals Heterostructures

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Abstract: Layer-by-layer assembly of van der Waals (vdW) heterostructures underpins new discoveries in solid state physics, material science and chemistry. Despite successes, all current assembly techniques use polymeric supports which limit their cleanliness, ultimate electronic performance, and potential for optoelectronic applications. In the first part of the talk, I will introduce a polymer-free platform for heterostructure assembly using re-usable flexible silicon nitride membranes. This approach enables production of heterostructures with interfaces free from interlayer contamination and correspondingly excellent optoelectronic behaviour. In addition, eliminating polymeric supports allows new possibilities for vdW heterostructure fabrication: assembly at temperatures up to 600°C, and in different environments including ultra-high vacuum and liquid submersion. In the second part, I will discuss how this new technology affects fabrication of twisted bilayer TMDs and extremely sensitive 2D materials such as magnetic tri- and di-halides. While UHV fabrication leads to quality improvement for all materials studied, we observe strong influence of surface conditioning and other fabrication steps and materials involved. In the last, conclusive part I will discuss the challenges the field is facing, using devices based on twisted 2D interfaces as an example. I will show the importance of nanofabrication in the context of twistrionics and offer avenues for future development of nanofabrication pathways.



Mechanism of Gold-Assisted Exfoliation

Jakob Ziewer^a, Abyay Ghosh^a, Michaela Hanušová^{b,c}, Luka Pirker^b, Otakar Frank^b, Matěj Velický^b, Myrta Grüning^a, and Fumin Huang^a

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Gold-Assisted Exfoliation (GAE) is a groundbreaking mechanical exfoliation technique capable of producing centimeter-scale, large-area monolayer crystals of two-dimensional (2D) materials [1]. In stark contrast, conventional exfoliation methods using Scotch tape and SiO₂/Si substrates typically yield micron-sized flakes—approximately six orders of magnitude smaller in area. The exceptional quality and scale of monolayers achieved via GAE have significantly advanced 2D materials research and enabled technological innovations, such as the fabrication of free-standing films, heterostructures, and moiré superlattices.

Since its inception, understanding the mechanism behind GAE—particularly its preference for generating monolayers over multilayers—has been a central focus of scientific inquiry. Prior studies highlight the adhesion between 2D materials and gold substrates as a critical factor. Research has established that successful exfoliation requires this adhesion to surpass the interlayer van der Waals forces within the 2D material. However, this alone does not explain why cleavage occurs preferentially at the first interface between the gold substrate and the adhered bottommost layer, rather than at other interlayer junctions.

In this study, we employ ultra-low frequency Raman spectroscopy to identify **strain-induced decoupling** as the primary mechanism governing GAE. Our findings reveal that in GAE systems, the coupling at the first interface (between the gold-adhered bottommost layer and its adjacent layer) is significantly weakened. For crystals exceeding five layers in thickness, the coupling at this interface is nearly eliminated, rendering it the weakest point in the structure. Consequently, exfoliation preferentially occurs here, yielding monolayers with lateral dimensions comparable to the parent crystal [2].

We attribute this decoupling effect to biaxial strain within the adhered layer, induced by the gold substrate. Density functional theory simulations further demonstrate that when the strain in the adhered layer and the crystal thickness surpass certain thresholds, monolayer exfoliation becomes energetically favorable.

References

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- [2] Jakob Ziewer, Abyay Ghosh, Michaela Hanušová, Luka Pirker, Otakar Frank, Matěj Velický, Myrta Grüning, and Fumin Huang, Strain-induced decoupling drives gold-assisted exfoliation of large-area monolayer 2D crystals, *Advanced Materials* 37 (2025), 2419184.

Investigating MBE growth and characterization of MoS₂ on Au(788) using ARPES and Raman Spectroscopy

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Semiconducting transition metal dichalcogenides (TMDC) are interesting due to their band structure in which the electron spin is coupled to the valley (K or K' point in 2D Brillouin zone) originating from inversion asymmetry and sizeable spin-orbit coupling. As a result, they are promising candidates for spintronics and valleytronics device applications^[1].

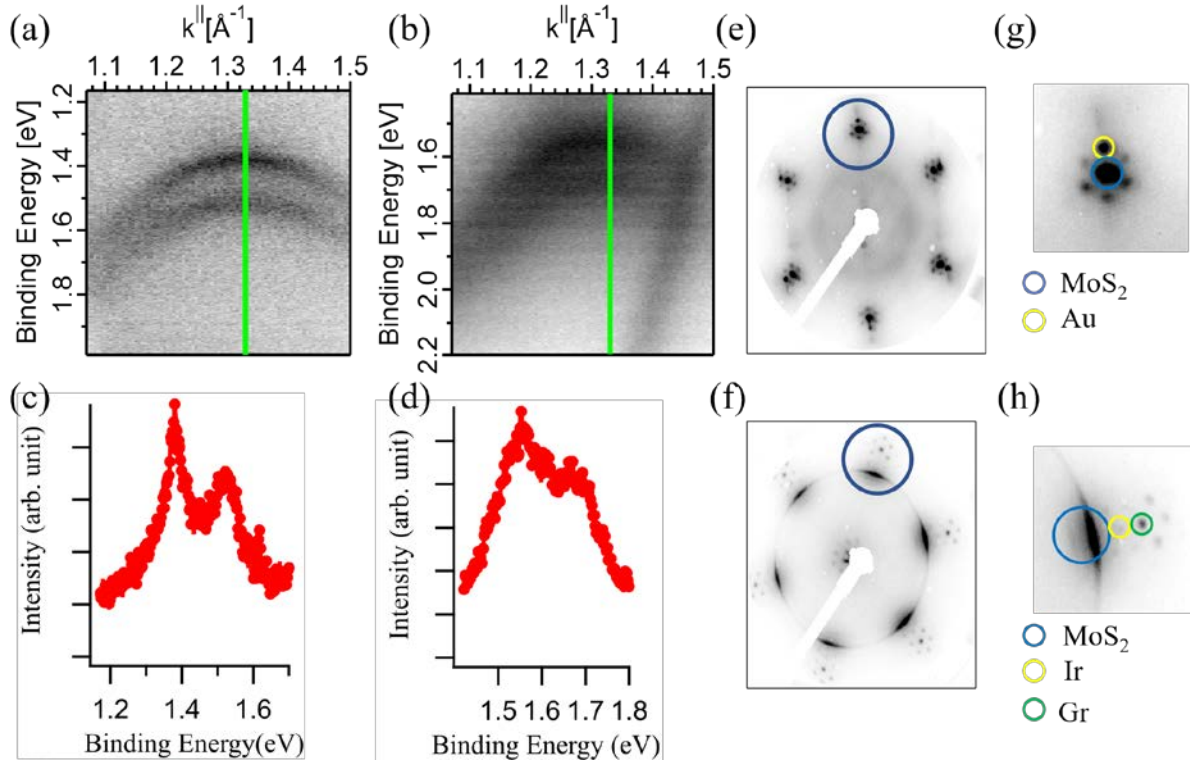


Fig: ARPES of ML MoS₂ on (a) Au(788) and (d) graphene/Ir(111) along Γ K direction where K point is indicated by green vertical line; EDCs at K point for MoS₂ on (b) Au(788) and (e) graphene/Ir(111); LEED of MoS₂ on (c) Au(788) and (f) graphene/Ir(111) and at 60 eV.

In the present work, we study the growth of monolayer MoS₂ on different substrates such as Au(788) and graphene/Ir(111) by molecular beam epitaxy^{[2][3]} based on van der Waals epitaxy^[4]. Sample growth quality is characterized using low-energy electron diffraction (LEED) and Raman spectroscopy. Furthermore, we transfer samples in vacuum to angle-resolved photoemission spectroscopy (ARPES) setup in order to investigate the electronic band structure. Analysis of the energy distribution curves (EDCs) and band broadening reveals superior crystalline and electronic quality of MoS₂ grown on the stepped Au(788) surface compared to the Gr/Ir(111)

substrate which further supports LEED measurement. Moreover, we interpret the results through theoretical modelling by tight-binding approach. In conclusion, our results introduce vicinal surfaces as a new substrate for growth of high quality TMDCs which makes a good platform to study spin-polarized states, effect of doping and intercalation on the optical and electronic properties of TMDCs.

References

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Band gap renormalization effects on electrochemical currents at 2D semiconductor/electrolyte interfaces

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One requirement for interfacial electron transfer reaction from a 2D semiconductor to molecules in solution is that the energy level of the electron in the semiconductor overlaps with the molecular acceptor energy levels in solution. The problem with emerging 2D semiconductor photocatalysts is that their energy levels are ill-defined relative to molecules in solution due to the band gap renormalization (BGR) effect. Monolayer (ML) transition metal dichalcogenides (TMDs) such as MoS₂ and WSe₂ exhibit giant BGR effects, where the electronic bandgap (E_g) dramatically changes with free carrier concentration (n), a quantity that changes with applied potential. Quantifying the BGR magnitude in electrochemical cells is critical for photo(electro)chemical solar energy conversion applications because efficient charge transfer depends on energy level overlap between the semiconductor and molecular electronic states. Here, using a combination of in situ spectroelectrochemistry and many body theory, we quantify the BGR effect magnitude for a ML MoS₂ electrode as a function of solution redox potential. Unlike bulk materials, the E_g of a ML MoS₂ electrode changes by over 200 meV upon varying the solution redox potential by 0.8 V. The BGR effect is driven by a charge equilibration process at the semiconductor-redox electrolyte interface that varies n ; charge equilibration stops when the Fermi level (E_F) of the semiconductor is equal to the redox potential of the solution phase. I will present cyclic voltammetry data that shows how BGR effects influence electrochemical currents. Our work pin-points key fundamental differences between bulk and ML semiconductor|redox electrolyte interfacial energetics and opens new avenues to tune electron transfer kinetics via the BGR effect. The second part of my talk will focus on solar energy conversion. The fundamental problem that limits the solar energy conversion efficiency of conventional semiconductors such as Si is that all absorbed photon energy above the band gap is lost as heat. The critical question that our research addresses is: Can we avoid energy losses in semiconductors? Ultrathin 2D semiconductors such as monolayer (ML) MoS₂ and WSe₂ have unique physical and photophysical properties that could make high-efficiency, hot-carrier energy conversion possible. Our research team has employed photocurrent spectroscopy, steady-state absorption spectroscopy, and in situ femtosecond transient absorption spectroscopy as a function of applied potential to characterize underlying steps in a ML MoS₂ photoelectrochemical cell. The rich data set informs us on the timescales for hot-carrier generation/cooling and exciton formation/recombination, as well as the magnitudes of changes in exciton energy levels, exciton binding energies, and the electronic band gap. These findings open the possibility of tuning the hot-carrier extraction rate relative to the cooling rate to ultimately utilize hot-carriers for solar energy conversion applications.

In-situ Raman (Spectro)Electrochemical Study of Intact and Defective Monolayer Graphene

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We present a localized microdroplet (spectro)electrochemistry setup for investigation of 2D materials, integrating in situ Raman spectroscopy with high resolution of the electrochemical measurements in micrometer-sized aqueous electrolyte droplets. This technique enables efficient electrolyte gating and voltammetry measurements, all complemented by in situ Raman spectroscopy. These capabilities provide valuable insights into the properties of 2D materials.

Localized experiments on monolayer graphene reveal differences in charge-transfer processes taking place at the basal plane and in defect-rich areas [1], enable the observation of Fermi level decay outside the electrochemically gated region, and show that gating efficiency is independent of the ionic electrolyte type in the high electrolyte concentration regime [2].

We will discuss the distinct behavior of the graphene G band in the Stokes and anti-Stokes regions at high electrochemical doping levels—a spectral region not previously accessed under such conditions. In this case, the influence of defects on the measured Raman response is ruled out. The data provide a new perspective on charge-transfer dynamics during electrochemical doping, offering fresh insights into the interplay between graphene's electronic structure and vibrational behavior, with applicability to other two-dimensional materials.

References

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Spatial Dynamics of the Fermi Level in Electrolyte-Gated Graphene

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Understanding how the electric field decays in monolayer graphene is critical for optimizing its performance in highly sensitive electronic applications, where precise control of the charge carrier density is required [1]. Our research examines the Fermi level dynamics in the basal plane of mechanically exfoliated monolayer graphene gated by an aqueous electrolyte. Our *in situ* experimental approach involves the concurrent but spatially distinct application of voltage *via* a microdroplet electrochemical cell, alongside Raman spectroscopy measurements. The frequency of the Raman G mode of graphene ($\Delta\omega_G$), serves as an indirect proxy to measuring the Fermi level of graphene.

We observe a rapid initial jump of the Fermi level towards the charge-neutral Dirac point upon crossing from the biased microdroplet interface to the unbiased dry graphene. This is followed by a more gradual equilibration of the Fermi level away from the microdroplet edge (Figure 1). Notably, the Fermi level does not fully return to its original undoped state within a distance of tens of micrometers from the gated microdroplet.

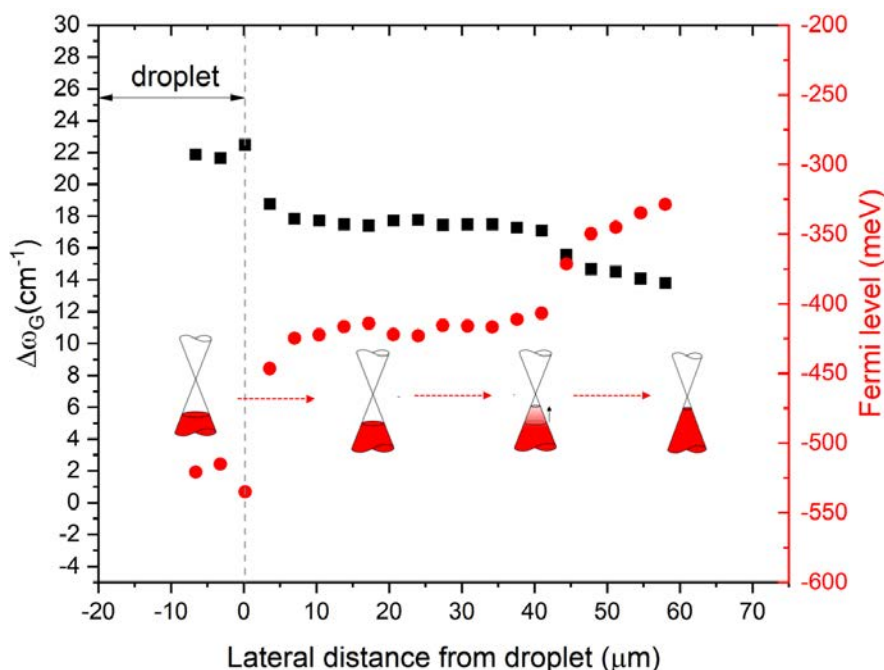


Figure 1. Evolution of $\Delta\omega_G$ (and therefore Fermi level) of monolayer graphene along the linear profile, from within the biased microdroplet region to the external unbiased region of dry graphene. The potential inside the droplet was held at +1.2 V (vs. Ag/AgCl in 6M LiCl).

References

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Exploring Resonance Raman Scattering and Stimulated Raman Scattering Effects in CrSBr

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Abstract:

CrSBr is an air-stable magnetic semiconductor and a van der Waals material with notable intrinsic properties, such as crystalline anisotropy, quasi-1D electronic behavior, and layer-dependent magnetism. In this talk, I will discuss the origin of the emission peak near 1.7 eV observed in its photoluminescence spectrum and the excitation energy-dependent Raman spectroscopy. I will also discuss the observation of stimulated Raman scattering (SRS) in CrSBr and CrSBr_xCl_(1-x) (0 < x < 0.5) highlighting the interplay between electronic and vibrational states in CrSBr and the Raman gain, which surpasses those reported in many three-dimensional systems. Additionally, I will comment on the unusually high anti-Stokes to Stokes intensity ratio in CrSBr, which varies with laser power and crystal orientation. These findings underscore the unique vibrational and electronic interactions and potential photonic applications of these material systems.

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Stability of transition metal thio(seleno)phosphate monolayers on gold substrates

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Transition metal thio(seleno)phosphate monolayers, including FePS₃, FePSe₃, and MnPS₃, are relatively stable materials that exhibit promising magnetic and electronic properties [1], [2]. However, their long-term environmental stability is limited. Bilayer FePS₃ on Si/SiO₂ substrate was reported to degrade after one week in ambient conditions [3]. Here we focus on the stability of these monolayers on gold substrates. While FePS₃ exfoliated in ultra-high vacuum (UHV) conditions onto Au/mica substrates, prepared by Ar⁺ sputtering followed by annealing, exhibits a signal in angular-resolved photoemission spectroscopy, the material exfoliated onto freshly prepared Au in air does not show any resolved signal. X-ray photoemission spectroscopy reveals major differences in S 2p core level shapes (Fig. 1), which we interpret as a fast degradation of the FePS₃ monolayer on gold exposed to air.

Our observations suggest that transition metal thio(seleno)phosphate monolayers on gold are much less stable compared to the layers on dielectric substrates. Understanding the substrate-dependent instability is essential for future applications of these materials in device technologies.

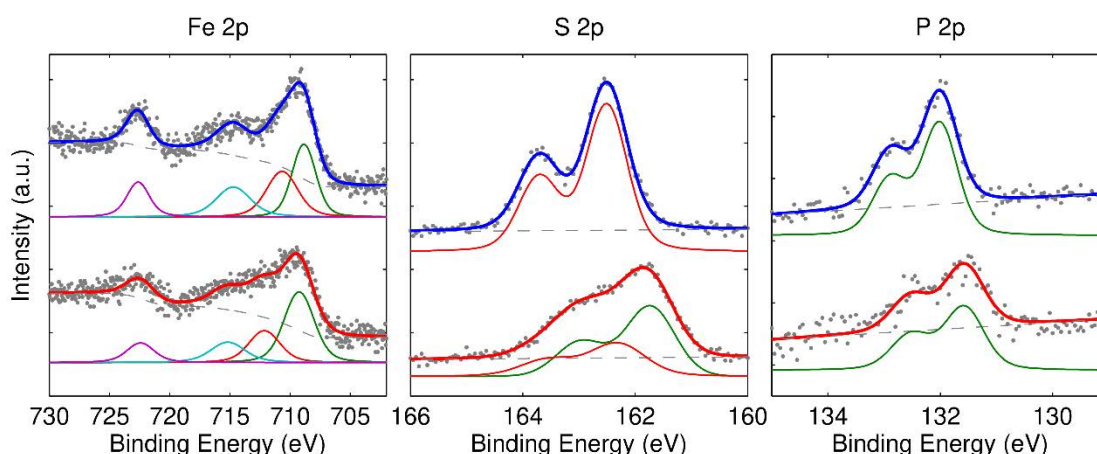


Fig. 1: Core levels of Fe 2p, S 2p, and P 2p of FePS₃ prepared in UHV (blue line) and in ambient conditions (red line).

References

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Sliding ferroelectricity in misfit layer compound (PbS)_{1.11}VS₂

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Twisted heterostructures of two-dimensional crystals can create a moiré landscape, thereby changing dramatically the properties of its parent crystals. The recent theoretical prediction [1] and experimental confirmation of sliding ferroelectricity [2,3] has significantly expanded the group of two-dimensional (2D) ferroelectrics. Due to the weak van der Waals interactions in layered van der Waals multilayers, an out-of-plane polarization can be created in many of those systems via in-plane interlayer sliding of a layer and thereby breaking the inversion symmetry.

Here, the alternated stacking of posttransition metal monochalcogenides and transition metal dichalcogenides in misfit layer compound crystals is used as a moiré generator. X-ray diffraction shows the presence of twins with a small twist angle between them. The surface electrical potential from the induced sliding ferroelectricity can be seen by using scanning probe microscopy and electron microscopy with domain sizes up to tens of micrometers.

Furthermore, I will show that generated moiré landscape in (PbS)_{1.11}VS₂ is a perfect playground to explore the properties of such moiré domains. For example, using electron-beam lithography, stable domains of arbitrary shape can be written or the catalytic activity of the micrometer large domains can be straightforwardly followed using optical microscopy to follow the growth of nanoparticles on the polarized domains.

References

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Controlling Wetting on Carbon Surfaces

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There has been considerable interest in, and debate over, the interactions between water and carbon surfaces, particularly for 1D and 2D forms of carbon. Anomalously high water fluxes have been reported in ultra-small channels formed from carbon nanomaterials, and the physical origin of these phenomena have been discussed [1,2]. Control over wetting with these surfaces is therefore important. Carbon materials are an ideal playground, therefore, to explore electrowetting, which is the potential-dependence of the contact angle of a liquid electrolyte on a solid substrate (electrode) [3]. Our most recent data has led to a re-evaluation of the classical Young-Lippmann methodology that has been used hitherto to interpret electrowetting data [4-8].

References

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Poster Session I (Monday)		
M1	J. Muthu	Polymer-Free, and Transfer-Free Fabrication of High Quality 2D Materials via Biphasic Iodine Etching
M2	F. Khurshid	Laser-Induced Chlorination of 2D Material
M3	C. Cheung	Clean assembly of van der Waals heterostructures
M4	Z. Dan	Ultra-high vacuum exfoliation method for the preparation of large-area single layer TMDC films
M5	M. Hanušová	Exploring the interaction of MoS ₂ with highly oriented gold surfaces
M6	D. Wang	Guided exchange-dipole spin wave in monolayer CrSBr
M7	F. Cîmpean	Ferroelectric Islands of hBN
M8	M. Hulman	Quest for proximity-induced superconductivity in thin PtSe ₂ layers
M9	V. Havránek	Ion beam micro-beam as a tool for modification of 2D materials

Polymer-Free, and Transfer-Free Fabrication of High Quality 2D Materials via Biphasic Iodine Etching

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The integration of two-dimensional (2D) materials into electronic devices is often hindered by contamination and structural degradation arising from polymer-assisted and mechanical transfer processes. To overcome these limitations, we introduce a universal, polymer-free, and transfer-free technique for the scalable integration of clean, large-area 2D materials. Our approach utilizes a biphasic iodine etching process applied to 2D flakes exfoliated onto gold-coated substrates via metal-assisted exfoliation. A sequential gas- and liquid-phase iodine treatment weakens the metal–2D interface and removes the underlying metal layer, enabling direct, residue-free integration of the 2D material onto dielectric substrates without manual transfer. This method is broadly compatible with various 2D semiconductors and provides a clean, scalable pathway toward high-performance device fabrication. The resulting devices exhibit improved material quality and electronic properties, offering a promising route for next-generation electronics and optoelectronics.



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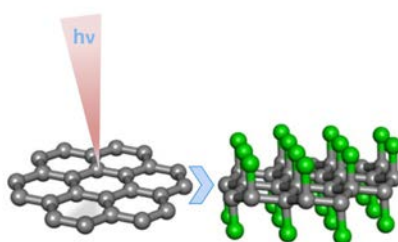
1. D. Wenlong, Z. Dai, L. Liu, Z. Zhang. Adv. Materials 36, no. 22 (2024) 2303014.

Laser-Induced Chlorination of 2D Material

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Chlorination of graphene presents significant challenges due to its unfavorable thermodynamics and weak surface interaction compared to fluorination. In this work, we report a novel method for the controllable chlorination of graphene using a 455 nm pulsed laser to generate reactive chlorine radicals from a solid chlorine-containing target. The laser parameters were carefully optimized to regulate the extent of chlorination with high spatial precision. The successful functionalization of graphene was confirmed through spatially resolved spectroscopy techniques, revealing uniform and tunable chlorine incorporation. Furthermore, we are developing a reversible (erasable) chlorination approach, which holds promise for reconfigurable electronic platforms such as artificial neural networks. This technique opens new avenues for atomically precise and dynamically reprogrammable graphene-based materials.



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Clean assembly of van der Waals heterostructures

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Two-dimensional crystals can be stacked layer-by-layer into heterostructures held by van der Waals forces possessing novel properties not seen in their constituent individual layers. However, most layer-by-layer assembly methods to date involve the use of polymeric supports, inevitably introducing contamination and limiting the operational conditions. Here, we present an inorganic assembly method based on flexible and transparent silicon nitride membranes coated with metal. Due to the non-use of polymers, these membranes can be used to transfer two-dimensional crystals under conditions that are previously inaccessible, including ultra-high vacuum, annealing at $> 200^{\circ}\text{C}$, and the use of aggressive cleaning techniques.

Heterostructures fabricated by this approach routinely demonstrate homogeneous contamination-free areas sized tens of micrometres. Additionally, transport measurements of encapsulated graphene devices assembled this way reveal exceptional carrier mobilities greater than $10^6 \text{ cm}^2\text{V}^{-1}\text{s}^{-1}$ at 4 K, suggesting a vast improvement in the device performance. We demonstrate this technique enables heterostructure assembly in ultra-high vacuum—a device fabricated in ultra-high vacuum exhibit ballistic transport over the scale of $> 40 \text{ }\mu\text{m}$, indicating the superior device quality thanks to ultra-clean device fabrication.

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Ultra-high vacuum exfoliation method for the preparation of large-area single layer TMDC films

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Two-dimensional transition metal dichalcogenides (2D TMDCs) have attracted significant attention as a potential platform for the next generation of electrical, optical and spintronic devices [1]. The prevalent method for preparing 2D materials, including 2D TMDCs, involves mechanical exfoliation using sticky tape [2]. This method produces 2D materials of highest quality, but they are usually small in size (tens of micrometers). In this context, we present our findings on the preparation of 2D WS₂ and WSe₂ using a recently developed kinetic *in situ* single-layer synthesis (KISS) method, which is performed in ultra-high vacuum and designed specifically for surface science research [3], Figure 1. The crystallinity and spatial morphology of 2D WS₂ and WSe₂ prepared on two distinct metallic substrates, Ag(111) and Au(111), using KISS method was investigated by X-ray photoelectron spectroscopy, low-energy electron diffraction, atomic force microscopy and X-ray standing waves (XSW). In particular, we focus on the influence that different substrates and chalcogen atoms have on the size and quality of exfoliated 2D films. We find that the quality of the bulk TMDC crystal, in this case WS₂ and WSe₂, plays a key role in the success of the KISS method exfoliation. Additionally, preliminary XSW measurements indicate that the KISS synthesis method does not compromise or diminish the quality of the underlying substrate, emphasizing its potential as a non-destructive approach for 2D material synthesis.

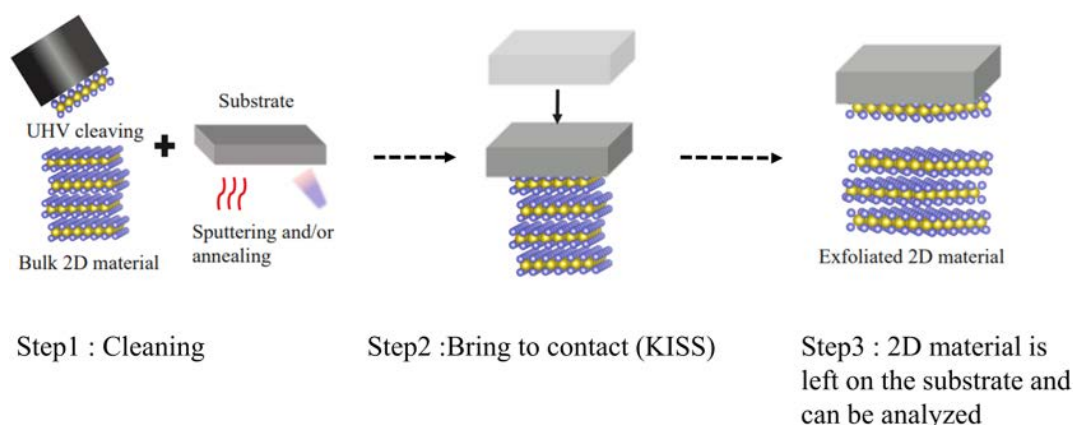


Figure 1. A schematic illustrating the KISS exfoliation procedure.

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Exploring the interaction of MoS₂ with highly oriented gold surfaces

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Gold-assisted exfoliation of transition metal dichalcogenides has gained significant interest due to its ability to produce high-yield, large-area monolayer flakes [1]. The electronic and vibrational properties of monolayer MoS₂ are highly sensitive to the underlying substrate, influencing its potential applications [2]. In this study, MoS₂ was exfoliated onto single crystalline gold surfaces: Au (111) and Au (100) under ultra-high vacuum conditions to ensure a pristine interface and prevent contamination.

The modifications induced by the substrate were analysed using angle-resolved photoemission spectroscopy and Raman spectroscopy, revealing distinct variations in the band structure and optical properties. Additionally, tip-enhanced Raman spectroscopy (TERS) provided nanoscale insights into local variation of the interaction (Fig. 1).

These findings underscore the role of the substrate crystal orientation in tuning properties of MoS₂ and offer deeper insights into the mechanisms governing metal-assisted exfoliation.

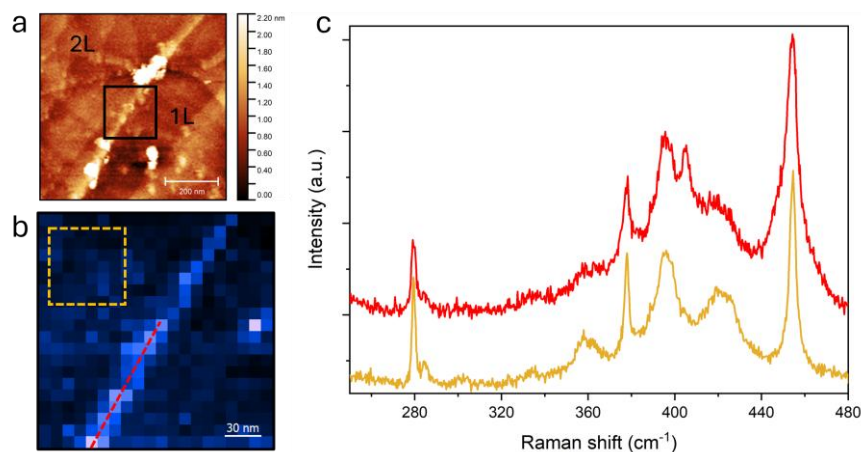


Figure 1: (a) Topography image of MoS₂ monolayer (1L) and bilayer (2L) exfoliated on Au (100) with the TERS map area defined by a black rectangle, (b) TERS map of the A_{2u} mode intensity (c) corresponding TERS spectra (obtained with 633 nm excitation) of the labelled areas in (b)

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Guided exchange-dipole spin wave in monolayer CrSBr

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CrSBr is an air-stable van der Waals antiferromagnet with high Néel temperature. We calculated the spin-wave spectrum for magnetization polarized along the three principal crystallographic axes 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. Due to the symmetry of the considered interactions, the spin-wave state is characterized by definite parity under space inversion. 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. Figure 1) with definite momentum. Effect of hybridization with acoustic phonons was investigated within the same framework. The 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.

The work was supported by the project Quantum Materials for Sustainable Technologies (QM4ST), no. CZ.02.01.01/00/22_008/0004572 funded by the MEYS and co-funded by the EU.

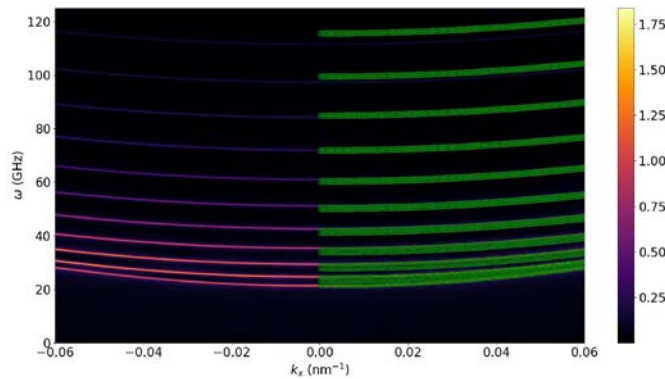


Figure 1. Theoretically calculated (green circles) and OOMMF simulated dispersion relation for a monolayer of CrSBr with magnetic field $B=0.7$ T applied perpendicular-to-plane. The dimension of the monolayer is $16384 \text{ nm} \times 256 \text{ nm}$.

Ferroelectric Islands of hBN

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Properties of novel van der Waals materials, including their conductivity and optical response, are dependent on the stacking order of their constituent layers. Therefore, control of the layer stacking order enables modulation of their intrinsic properties. One system that demonstrates this is the sliding of hBN layers with respect to one another, which gives rise to structures of alternating ferroelectric polarization polytypes AB or BA. These polytypes are mirror-symmetric and switch between one another both by mechanical translation as well as when an external electric field is applied. Isolated islands of ferroelectric hBN have been investigated by Yeo *et al.*^[1] using a cavity array enabled through the use of a spacer. They induce ferroelectric switching using an external electric field. In this work, hBN spacers (2-4 nm thick) with an array of etched cavities are encapsulated by parallel hBN crystals and their ferroelectric response is investigated. The top hBN crystal sags into the spacer cavities, creating contact islands of different polytype domains. The ferroelectric response at these contact interfaces is characterised using EFM and PFM and the potential of manipulating the size and distribution of the ferroelectric domains within these cavities is investigated. Utilising hBN spacers, rather than the graphene spacers used in the referenced previous work, removes interference from screening effects, improving the observation of the ferroelectric domains.

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Quest for proximity-induced superconductivity in thin PtSe₂ layers

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Proximity-induced superconductivity in transition metal dichalcogenides (TMDs) provides a versatile platform for investigating unconventional superconducting states and topological phenomena. TMDs such as WTe₂, with strong spin-orbit coupling and non-trivial band topology, are promising candidates for realizing topological superconductivity. The proximity effect enables the induction of Cooper pairing in these materials without modifying their intrinsic electronic structure, allowing for the emergence of exotic quantum states, including Majorana zero modes and one-dimensional topological superconductivity [1].

Previous studies have demonstrated long-range superconducting coherence in WTe₂ (up to 7 μm), coexistence of superconductivity with helical edge states [2], and transport anomalies attributed to the material's Weyl character [3].

These experiments typically employed serially stacked NbSe₂/WTe₂ heterostructures with overlapping flakes and four-probe measurements using in-plane current and voltage contacts.

Our work presents an alternative approach based on a vertical heterostructure consisting of a superconducting NbN layer and a thin PtSe₂ film. PtSe₂ was selected for its excellent chemical and environmental stability. While intrinsic superconductivity in PtSe₂ has only been theoretically predicted—with a critical temperature well below 1 K—we observe the onset of a superconducting state at a temperature nearly identical to that of the NbN layer, suggesting a proximity-induced effect (see Fig.1). The large sample area ($\sim 1\text{ cm}^2$) allowed us to investigate both two- and four-probe configurations. These findings may provide a pathway for exploring proximity effects in chemically stable TMDs with clean vertical interfaces.

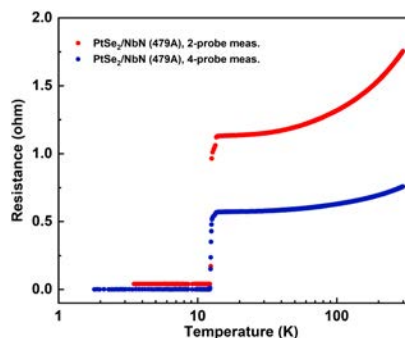


Fig. 1. Temperature dependence of resistance for vertically stacked layers of NbN and PtSe₂. The critical temperature is the same for 2-probe and 4-probe measurements, but the resistance below T_c varies for these configurations.

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Ion beam micro-beam as a tool for modification of 2D materials

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The energetic ion beams has a unique capability in modification and changing the functionality of 2D materials [1]. It can change its morphology, chemical composition, create specific defect in crystalline structure or dope specific atoms into the material. When using focused beam, this can be done also on preselected specific pattern with microscopic resolution. The variety of ion species, wide range of ion energies and experiment design can help to achieve desired properties with high efficiency.

The Ion micro-beam line at NPI is situated at +10deg line of 3MV TANDETRON 4130MC electrostatic accelerator and it is in operation since 2009. Routinely we have focused H, He, C, N, O beams in MeV energy range down to 1-2 μ m in high current mode (1-300 pA), when we can obtain doses up to 1e16 atoms per cm² in reasonable time. On the other hand we can reduce the current down to few ion per second (low current mode) with even better focusing (300-500nm beam spot). This mode can be used for single ion modification of material at specific place or pattern [2]. The same procedure can be used also for 2D material modification. The micro-beam target chamber is now equipped with precise 3D piezoelectric positioning stage with submicron resolution and full 360 deg. step motor rotation with 0.05 deg. step resolution. This, together with electromagnetic scanning unit, allows us to irradiate sample at any position and selected angle of incidence.

Another example of using focused ion beams is a formation of conductive micro tracks in graphene oxide foils [3] by MeV He ions. The deposited ion energy mainly is released as electronic energy loss. It leads to chemical bond breaking, free radical formation, ionization and excitation effects, heating and desorbing of functional oxygen groups and water molecules, which enhance the electrical conductivity of the rGO proportionally to the ion fluence used. Other ions as C or O can be also utilized.

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- Testing Chambers for Climatic and Temperature Testing

Tuesday, June 10

7:00-9:00	Breakfast		
9:00	Morning session:		
<i>Time</i>	<i>Chair</i>	<i>Speaker</i>	<i>Title of presentation</i>
9:00-9:40	P. Kusch	D.R.T. Zahn	Tip-enhanced Optical Spectroscopies for Studying 2-dimensional Semiconductors and their Interfaces
9:40-10:00		A. Fiocco	Proximity-induced "magic" Raman bands in TERS spectra of MoS ₂ and WS ₂ deposited on the 1L h-BN-capped gold
10:00-10:20		L. Lafeta	Tip assisted Fourier space nonlinear images of 2D Materials
10:20-10:40		K. Salamon	Atomic defect behaviour in magnetic transition metal dihalides
10:40	Coffee break		
<i>Time</i>	<i>Chair</i>	<i>Speaker</i>	<i>Title of presentation</i>
11:10-11:50	A. Grubišić-Čabo	C. Casari	Pulsed Laser Deposition of 2D TMDs on Metals: from large area Monolayers to Heterostructures
11:50-12:10		J. Honolka	Occupied and unoccupied band structure studies of MoS ₂ monolayers on Au(111) using angle-resolved photoemission and inverse photoemission methods
12:10-12:30		L. Pirker	The Role of Metallic Substrates in Large-Area Exfoliation of TMDCs
12:30	Lunch		
14:30	Afternoon session:		
<i>Time</i>	<i>Chair</i>	<i>Speaker</i>	
14:30-14:50	D.R.T. Zahn	C. Soe	Metal-Assisted Exfoliation of MoS ₂ : The Role of Au Roughness on Optical and Vibrational Properties
14:50-15:10		F. Karlický	Optical and Excitonic Properties in 2D Materials and van der Waals Heterostructures Using Many-Body Methods
15:10-15:30		E. Paiva de Araujo	Fabrication and Characterization of Janus Transition Metal Dichalcogenide
15:30-15:50		P. Markus	Advancing Nanoscale Material Characterization with AFM: Innovations in Electrical Properties Mapping
15:50	Coffee break + Poster session II		
<i>Time</i>	<i>Chair</i>	<i>Speaker</i>	<i>Title of presentation</i>
17:20-18:00	C. Casari	P. Kusch	Surface Exciton Polaritons in 2D Transition Metal Dichalcogenides
18:30	Buffet dinner		

Tip-enhanced Optical Spectroscopies for Studying 2-dimensional Semiconductors and their Interfaces

Dietrich RT Zahn

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Two-dimensional (2D) semiconductors are among the most extensively studied materials showing potential in a large spectrum of applications from electronics/optoelectronics to photocatalysis and CO₂ reduction. These materials possess astonishing optical, electronic, and mechanical properties, which are different from their bulk counterparts. Due to strong dielectric screening, local heterogeneities such as edges, grain boundaries, defects, strain, doping, and chemical bonding dictate their physical properties to a great extent. Therefore, there is a growing demand of probing such heterogeneities and their effects on the physical properties of 2D semiconductors on site in a label-free and non-destructive way. Tip-enhanced Raman spectroscopy (TERS), which combines the merits of both scanning probe microscopy and Raman spectroscopy, has experienced tremendous progress since its introduction in the early 2000s and is capable of local spectroscopic investigation with nanometer spatial resolution. Applying this technique to 2D semiconductors not only enables us to understand the effects of local heterogeneities, it can also provide new insights opening the door for novel quantum mechanical applications.

In this contribution, we deliver a short introduction to the most commonly used 2D semiconductors, namely the transition metal dichalcogenides (TMDCs), and their properties. Subsequently we briefly introduce the basics of TERS as well as tip-enhanced photoluminescence (TEPL). Then we discuss several examples highlighting the application of tip-enhanced optical spectroscopies (TEOS) to 2D semiconductors.

Optical and Excitonic Properties in 2D Materials and van der Waals Heterostructures Using Many-Body Methods

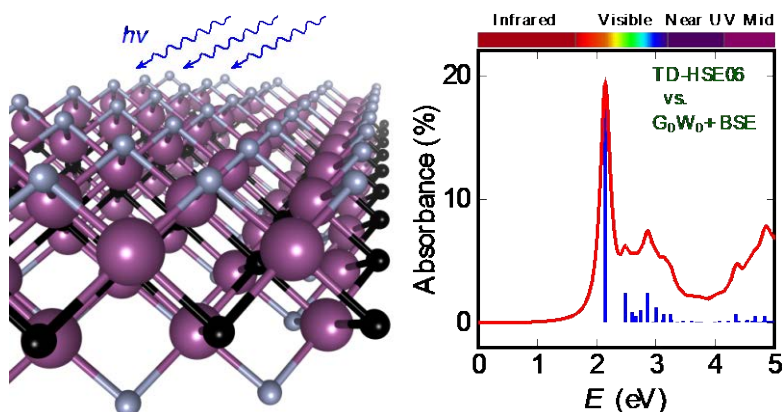
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Electron-electron and electron-hole (exciton) effects are specifically pronounced in two-dimensional (2D) materials because of weak dielectric screening from the environment. Many-body GW approximation and Bethe-Salpeter equation (BSE) are considered state-of-the-art methods for reliable prediction of fundamental [1-2] and optical [3-4] gaps of various 2D materials. Although the well-converged GW+BSE approach can predict such delicate phenomena as the excitonic insulator [5], it's still very demanding concerning computational time and memory used and its usage for a larger supercell is almost unfeasible. We recently proved that time-dependent density functional theory (TD-DFT) based on specific screened hybrid density functional can effectively account for all important physical effects, including excitons [6-7], thus, it is a practicable technique for van der Waals heterostructures containing incommensurate cells of different monolayers and enables detailed analysis of intra- and interlayer excitonic wave functions [8].

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Tip assisted Fourier space nonlinear images of 2D Materials

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Fourier-space imaging offers a powerful means to probe the angular emission patterns of optical sources, revealing key information about material properties such as crystal symmetry and orientation. In particular, Fourier second-harmonic generation (FSHG) has proven effective for characterizing two-dimensional (2D) materials [1]. However, like other far-field optical techniques, its spatial resolution is restricted by the diffraction limit. To overcome this limitation, tip-enhanced methods, successfully applied in photoluminescence (TEPL) [2] and Raman spectroscopy (TERS) [3], have been explored for nonlinear optical processes such as second-harmonic generation (TESHG) [4]. Despite their potential, TESHG techniques face significant challenges, especially due to the strong nonlinear far-field background from both tip and sample, which reduces the signal-to-noise ratio of the near-field component. In this work, we analyze TESHG in Fourier space to distinguish the localized near-field signal from far-field background contributions. Based on dipole emission modeling, we demonstrate that these components produce distinct radiation patterns in Fourier space, enabling their separation, as illustrated in Figure 1.

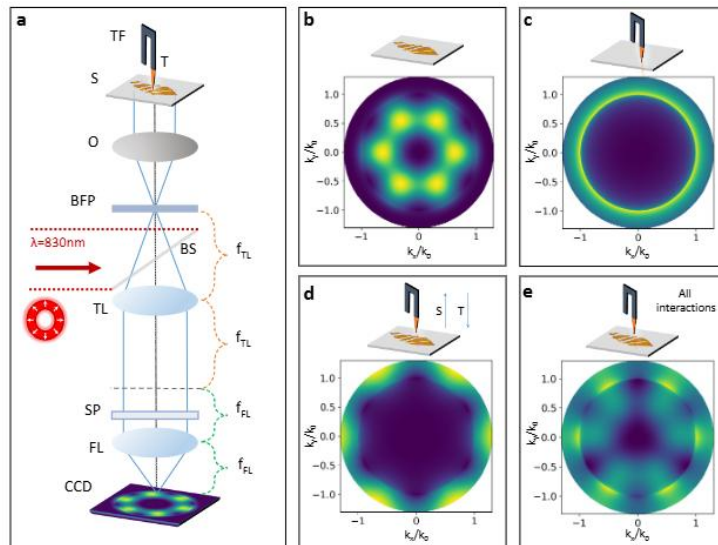


Figure 1: **a)** Schematic of the 4f optical system used to project the Fourier space image onto the CCD detector. **b)** Simulated Fourier-space SHG pattern generated by a sample with D_{3h} symmetry under radial polarization. **c)** Fourier-space pattern generated by a tip-only configuration (modeled as a z-oriented dipole). **d)** Tip-enhanced SHG signal radiated by the sample upon localized excitation. **e)** Combined SHG signal resulting from the interference of the sample, tip, and tip-enhanced contributions.

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Proximity-induced “magic” Raman bands in TERS spectra of MoS₂ and WS₂ deposited on the 1L h-BN-capped gold

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The nanoscale resolution of tip-enhanced Raman scattering (TERS) makes it a powerful tool to image and identify structural properties and defects in 2D semiconductors. Recently, we proposed an “ideal” substrate for gap-mode TERS and tip-enhanced photoluminescence (TEPL), namely 1L h-BN-capped gold or silver [1]. We fabricated such gold-based substrates and demonstrated a strong TERS and TEPL response from a WS₂ monolayer, exfoliated on it. Unexpectedly, in addition to the Raman bands of WS₂, we observed strong narrow bands (at ~76 cm⁻¹ and ~796 cm⁻¹) that normally do not appear in the Raman spectra of either WS₂ or h-BN. Since these bands were observed in the same spectral position in the TERS spectra of MoS₂@1L h-BN@Au, it became clear that they originated from h-BN. The literature search [2,3] showed that a similar effect was observed in the far-field Raman spectra of h-BN-encapsulated WSe₂. However, in our case the dependence of the intensity of the “magic bands” on the excitation laser wavelength was completely different, strongly resembling the one of the A'/A_{1g} ratio of WS₂@Ag [1], with the magic bands disappearing at the excitation laser energy corresponding to A exciton in WS₂. We will here discuss possible origins of these magic bands, as well as the nature of such unexpected excitation wavelength dependence.

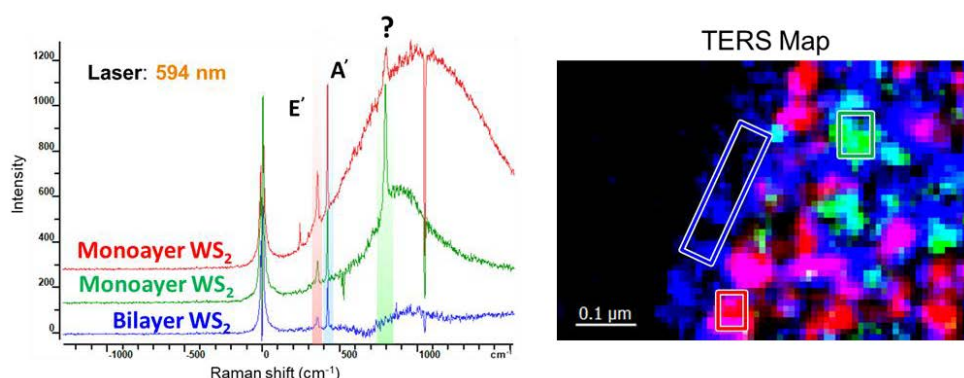


Figure: TERS spectra (left) averaged from a hyperspectral map (right) of WS₂@1L h-BN@Au.

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Pulsed Laser Deposition of 2D TMDs on Metals: from large area Monolayers to Heterostructures

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Transition metal dichalcogenides (TMDs) are emerging semiconductors for 2D electronics, optoelectronics, catalysis, and energy storage. Understanding the interaction between 2D TMDs and various substrates, as well as controlling the fabrication of vertical and lateral TMD heterostructures, is critical for engineering functional layered systems. In this framework the physics at TMD interfaces play a crucial role with many challenges when synthesis techniques beyond mechanical exfoliation are employed.

Here, we discuss how pulsed laser deposition (PLD) in UHV and thermal annealing are exploited to grow MoS₂ and WS₂ layers with finely controlled coverage, from 2D nanoislands, to large area single-layers (SL) and to few-layers and multi-layer films, on metallic substrates, e.g. Au(111) and Ag(111), and inert substrates, (e.g. SiO₂/Si or glass) [1-3].

The epitaxial growth of SL TMD on metal substrates is investigated by in situ scanning tunneling microscopy (STM), showing a polycrystalline structure and a distinctive moiré pattern [1]. Raman spectroscopy reveals a strong interaction with the metal substrate, dependent on the type and orientation of the surface, attributed to substrate-induced doping and strain [4].

Vertical heterostructures consisting of TMD hetero-bilayers (HBL) (i.e. MoS₂/WS₂ or WS₂/MoS₂) and lateral hybrid heterostructures between PLD-grown SL MoS₂ nanoislands and pentacene molecule on metal substrates are discussed [5,6]. The combined use of STM/STS and Raman spectroscopy provides information on the layer-by-layer growth, TMD-substrate interactions, stacking order effects and interlayer coupling. A custom wet-etching transfer procedure allows us to transfer PLD-grown films and hetero-bilayers from metal surfaces to SiO₂/Si substrates, thus enabling to decouple them from the native substrate. We observe a sharp change in the density of states across the pentacene/MoS₂ lateral interface, indicating a weak interfacial coupling and abrupt interface.

These results highlight the potential of PLD as a method to grow TMD based heterostructures, opening to new perspectives in the synthesis of complex 2D layered materials towards possible device implementation.

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Occupied and unoccupied band structure studies of MoS₂ monolayers on Au(111) using angle-resolved photoemission and inverse photoemission methods

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It is known that exfoliation of transition metal dichalcogenides onto, or assisted by, an Au(111) surface is able to result in large-scale single-domain samples of several millimeters in diameter, often with remarkable homogeneous quality. While the occupied electronic band structure is nowadays accessible even down to micrometer-scale samples by micro-ARPES methods, angle-resolved inverse photoemission spectroscopy (ARIPS) studies [1] of unoccupied bands usually require much larger sample areas.

Here we report on ARIPS and ARPES results on the unoccupied & occupied band structure and work function values derived from exfoliated, large-scale MoS₂ monolayer areas on Au(111) with a finite twist-angle. A comparison with literature results, e.g., from bottom-up grown MoS₂ monolayers on Au(111) with twist angles close to zero [2,3] and twist-angle dependent DFT calculations is done.

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

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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 MoS₂/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 MoS₂ and offer key insights into the mechanisms driving metal-assisted exfoliation.

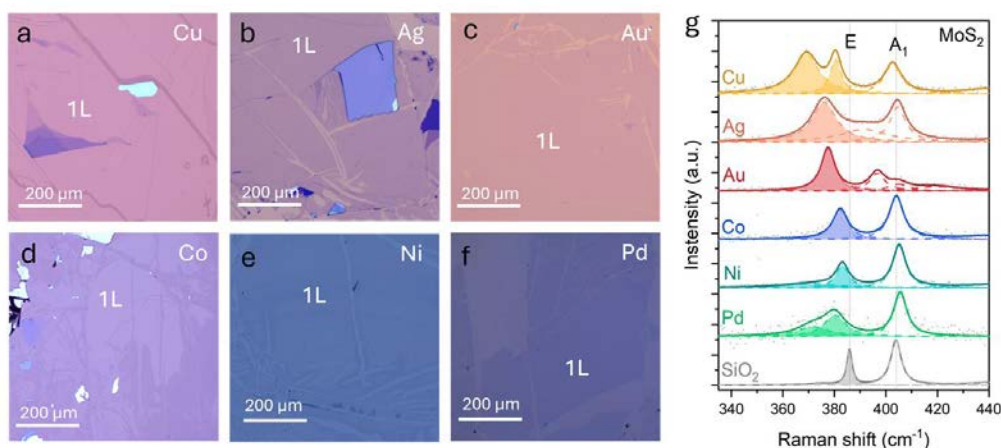


Figure 1. (a-f) Optical images of large-area MoS₂ monolayers exfoliated on Cu, Ag, Au, Co, Ni, and Pd. (g) Raman spectra of MoS₂ monolayers exfoliated on different metals.

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Metal-Assisted Exfoliation of MoS₂: The Role of Au Roughness on Optical and Vibrational Properties

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Gold-assisted exfoliation has become an outstanding technique for producing large-area monolayers of transition metal dichalcogenides (TMDCs), enabling the study of TMDC-gold interfaces, moire potentials, charge density wave, and band structure modifications(1-3). Despite prior studies on the interaction between molybdenum disulfide (MoS₂) and gold (Au), the influence of roughness on the optical and vibrational properties of MoS₂/Au heterostructures remains unclear. In this work, we investigate the interaction between monolayer MoS₂ exfoliated on Au of varying thickness, deposited on silicon dioxide (SiO₂) wafer using magnetron sputtering. We characterize the topography and roughness of both the Au substrates and the exfoliated MoS₂ monolayers. Our Raman spectroscopy analysis reveals a consistent splitting of the out-of-plane (A₁) mode across all thicknesses. Furthermore, in samples exhibiting significant roughness, we observe the splitting and downshift of the in-plane (E) mode, which is correlated with a downshift of the A₁(L) mode. For certain thickness, we observe the appearance of photoluminescence (PL), which is correlated with the topography of the MoS₂ surface. Polarized Raman measurements in cross-polarization show a non-vanishing contribution of the A₁ mode, which is correlated with the roughness and geometry of the MoS₂ surface. The samples were further investigated with Kelvin Probe Force Microscopy and tip-enhanced PL revealing the nanoscopic origin of the emission. Furthermore, the tip-enhanced Raman spectroscopy was employed to investigate the origin of the correlation between the A₁ and E modes.

Keywords: MoS₂ roughness, gold roughness, Raman spectroscopy, interaction

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Atomic defect behaviour in magnetic transition metal dihalides

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Scanning transmission electron microscopy (STEM) is a powerful tool for characterizing the atomic structure of materials. However, its application to highly air sensitive 2D materials such as 2D transition metal halides has been limited due to challenges in sample fabrication. In this study, we developed a novel inorganic stamping based method, using silicon nitride membranes[1] to fabricate pristine suspended 2D material samples suitable for STEM analysis. This technique enables hermetic encapsulation of extremely air-sensitive 2D materials by protecting them with graphene layers on both sides. The simple, fast and polymer free technique causes no mechanical damage to the sample, preventing degradation due to minor imperfections in the seal. Using this method, we structurally characterized transition metal dihalides (FeI_2 , NiI_2) across various thicknesses, from bulk to monolayer structures for the first time. We observed a thickness dependent stacking transition in FeI_2 , where the preferred arrangement changed from bulk 1T stacking to bilayer 3R stacking. Additionally, we showcase the stability of the as-transferred materials by analysing the formation of atomic vacancies and spontaneous in situ study of the regrowth of monolayer FeI_2 during prolonged electron beam irradiation at one nanopore. Real-time observation of the healing of defects at atomic resolution can help to achieve controlled repair of various damages in 2D materials starting from monovacancy to more complex defects. Our work demonstrates the potential of this transfer technique not only for enabling efficient advanced TEM characterisation (and complementary techniques which require suspended samples) of previously inaccessible air-sensitive thin 2D materials, but also for new approaches to tailoring 2D materials in the future with specific structures for various applications.

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Fabrication and Characterization of Janus Transition Metal Dichalcogenide

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Janus 2D Transition Metal Dichalcogenide (TMD) is formed by two different chalcogen atoms on each side of the metal plane (represented as Janus XMY, where M = transition metal; X = chalcogen at the bottom; Y = chalcogen at the top). Due to this broken out-of-plane mirror symmetry and electronegativity difference between top and bottom layers, Janus TMDs exhibit internal perpendicular electric field, which leads to an occurrence of variety of novel physical phenomena. In this study, we have observed the hexagonal TMDs, namely MoSe₂ and WSe₂ during the sulfurization process, with the aim to fabricate Janus MoSSe and WSSe structures, respectively. The reaction was carried out inside the scanning electron microscope (SEM) chamber, equipped with a custom-build chemical vapour deposition (CVD) gas delivery system. This setup allows to use of H₂S gas as a sulphur source for selective substitution of selenium atoms. In-situ SEM experiments have shown that it is possible to observe morphological changes induced by high temperature, as well as to track the chalcogen exchange process in both monolayer and multilayer materials. Raman spectroscopy confirmed the presence of Janus structure, showing that these stackings are more easily formed in multilayer systems than in monolayers. Additionally, for monolayers, photoluminescent spectra showed quenching where defects were present due to the absence of chalcogenide atoms, as well as emergence of a mixture of states (WS_{2(1-x)}Se_(2x)) that appeared at high temperatures, instead of a well-defined Janus monolayer.

Advancing Nanoscale Material Characterization with AFM: Innovations in Electrical Properties Mapping

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The behavior and properties of modern materials are intricately linked to their structural, mechanical, and electrical characteristics at the nanoscale. Atomic Force Microscopy (AFM), with its exceptional x-, y-, and z-resolution, has become a pivotal tool for investigating these properties. Beyond 3D topographical imaging, AFM offers a diverse range of measurement modes that enable the correlation of topography with material-specific properties. The DriveAFM, recently introduced by Nanosurf, represents a significant advancement in AFM technology. This tip-scanning AFM combines high-performance measurement capabilities with fully motorized system integration. Leveraging the CleanDrive photothermal excitation technology, the DriveAFM enables faster imaging and opens new possibilities for measuring electrical interaction forces. In this talk, we will demonstrate how the technological innovations of the DriveAFM enhance ease of use and support a variety of nanoscale electrical characterization techniques. Highlighted examples include recent advancements in conductive AFM, Kelvin probe force microscopy (KPFM), and scanning microwave microscopy (SMM). These methods facilitate the mapping of local conductivity, surface potential, permittivity, charge carrier density, and other critical properties, showcasing the DriveAFM's potential to advance nanoscale material characterization.

Surface Exciton Polaritons in 2D Transition Metal Dichalcogenides

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In recent years, two-dimensional transition metal dichalcogenides (TMDCs) have been extensively studied due to their ability to host excitons at room temperature. This enables tunable optical and electronic properties with promising applications, such as single-photon emitters.

A powerful tool for studying TMDC properties is scattering-type scanning near-field optical microscopy (s-SNOM). It provides information on the dielectric function while operating far below the diffraction limit of light. Imaging via s-SNOM uses a sharp metallic tip of an atomic force microscope (AFM) to enhance incoming and scattered light by excited near-fields at the tip apex leading to high sensitivity and a spatial resolution of a few nanometers. Furthermore, s-SNOM enables excitation and imaging of propagating polaritons in real space.

Polaritons, arising from light-matter coupling, are particularly significant in TMDCs, where light couples with excitons, resulting in exciton-polaritons. We showed imaging and dispersion mapping of these novel quasi-particles in MoS₂ and WS₂ slabs as thin as 10 nm using s-SNOM [1]. The imaging in Ångström-thin samples remains challenging due to the refractive index requirements of the cladding media. Initial studies indicate that modes may persist in TMDC monolayers with symmetric dielectric environments[2]. While photoluminescence confirms propagating modes, their real-space visualization and dispersion remain unexplored. We will explore exciton-polaritons in a freestanding WS₂ monolayer by imaging their real-space propagation using s-SNOM. Fig. 1 (a) and (b) shows an example of propagating polaritons. We obtain the polariton dispersion relation, which exhibits at least strong light-matter coupling around the binding energies of the A and B excitons. Through modeling the dispersion of a TE₀ mode in monolayer WS₂, we identified the excited polariton as a surface exciton-polariton. This surface quasi-particle had been theoretically predicted for TMDCs but has not been experimentally observed due to technical challenges.

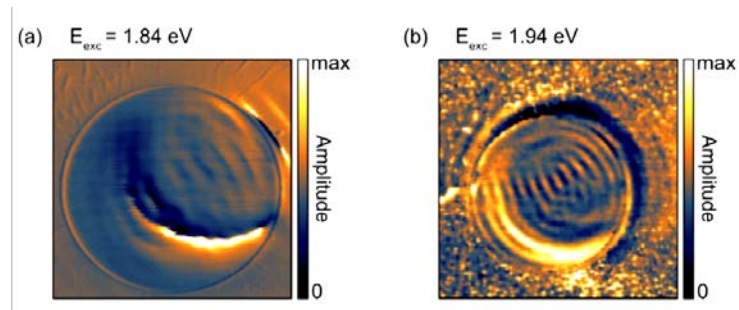


Fig. 1 Real space images of propagating polaritons in a free-standing monolayer of WS₂. In (a) the TMDC is exfoliated onto a hole drilled into SiN and excited at 1.84 eV in (b) on gold and excited at an energy of 1.94 eV.

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Poster Session II (Tuesday)		
T1	M. Žáček	Exploring Opto-Spintronic Behavior in van der Waals Magnetic Devices
T2	S. Keszei	Investigating MoS ₂ catalysts with Scanning Electrochemical Cell Microscopy (SECCM)
T3	J. Kalbáčová Vejpravová	Light-Mater Interaction in 2D Magnets: Key Concepts and Future Directions
T4	A. Kayal	Study of Photoluminescence in He ⁺ -ion irradiated MoS ₂
T5	M. Kalbáč	UHV exfoliation of 2D materials
T6	P. Čech	Localized Raman Spectroelectrochemistry in an All-Iron Aqueous Redox Flow Battery System
T7	J. David	LEEM Observation of Graphene Intercalation O ₂ , CO, H ₂ , H ₂ O and CO ₂
T8	Z. Vlčková	Raman spectroelectrochemical Insights into Doped Diamond Electrodes in Water-in-Salt Electrolytes
T9	S. Ghosh	Optimising growth parameters for 2D transition-metal dichalcogenides using chemical vapour deposition

Exploring Opto-Spintronic Behavior in van der Waals Magnetic Devices

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Two-dimensional (2D) materials have opened new opportunities in optoelectronics and spintronics, particularly in controlling electronic properties by interaction with visible light. With our Hall bar-based device made from the CrSBr magnet, we demonstrate how polarized light effectively manipulates the magnetotransport response. Our study confirmed previous results and uncovered additional phenomena that highlight the significance of light-matter interactions in CrSBr. We observed substantial light-induced enhancement of magnetoresistance ratio (MRR) and current polarity-dependent MRR.

These findings reveal the complex nature of light-matter interactions in magnetic 2D materials, such as CrSBr and expands the potential of magnetic van der Waals materials for future opto-spintronic applications.

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Investigating MoS₂ catalysts with Scanning Electrochemical Cell Microscopy (SECCM)

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Electrocatalytic hydrogen production has the potential to meet the increasing demand for hydrogen; however, its viability depends on the development of cost-effective and efficient electrocatalysts. MoS₂ nanocrystals are well-known for their catalytic activity in the hydrogen evolution reaction (HER), although only the edges are considered catalytically active sites, while the pristine surfaces of these 2D crystals are known to be inert. This duality creates a demand for activating the basal plane sites, which can be achieved through the introduction of various defects, imperfections, or chemical modification of basal plane sulphur atoms. Unfortunately, conventional electrochemical investigations typically provide only an average measure of the catalytic activity of samples, lacking insight into the behaviour of diverse surface features, such as crystallites with varying morphologies, grain boundaries, point defects, wrinkles, and other lattice imperfections. Scanning Electrochemical Cell Microscopy (SECCM) is an emerging technique that provides valuable information about the nature of the most active sites, enabling electrochemical measurements with high spatial resolution. Here we present our most recent results on various 2D transition metal dichalcogenide (TMDC) crystals using SECCM measurements. Monitoring the overpotential of the well-defined one electron reduction of [Ru(NH₃)₆]³⁺ allowed the investigation of local charge transfer characteristics, while voltametric measurements in strongly acidic medium provided direct information about the local catalytic activity of the samples, achieving a resolution of approximately 100 nm. Highly active surface sites can be correlated with atomic resolution structural data obtained by Scanning Tunneling Microscopy measurements, that will allow us to identify the true active sites of pristine and modified 2D TMDC crystals.

Light-Matter Interaction in 2D Magnets: Key Concepts and Future Directions

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Light-matter interactions in two-dimensional (2D) magnetic materials offer a powerful platform for probing and manipulating their electronic, spin, and symmetry-driven properties [1-3]. Optical spectroscopies, including Raman scattering, photoluminescence (PL), and magneto-optical Kerr effect (MOKE) measurements, reveal the intricate coupling between photons and spin-dependent excitations. These techniques enable the study of magnetic ordering, phase transitions, and anisotropic interactions, providing valuable insights into the fundamental behaviors of these materials. The interplay between light polarization and symmetry selection rules plays a crucial role in governing exciton and magnon resonances, which further illuminates the underlying electronic and magnetic structures of 2D magnets. By utilizing polarization-resolved spectroscopic techniques, it becomes possible to distinguish symmetry-allowed and symmetry-forbidden transitions, revealing hidden degrees of freedom that influence the material's properties.

In this contribution, I will summarize the state of the art in the field, highlight recent advances in understanding the light-matter interactions driving correlated phenomena in 2D magnets, and discuss several key examples that demonstrate their potential for future spintronic and quantum applications, relevant to the AMULET (Advanced MULTiscale materials for key Enabling Technologies) project.

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Study of Photoluminescence in He⁺-ion irradiated MoS₂

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Defect engineering in two-dimensional (2D) materials has been one of the most attractive routes for tuning their optical and electronic properties. Though intrinsic defects in TMDCs are detrimental to their optical emissions, significantly suppressing the PL by introducing a non-radiative decay channel, precisely engineered, localized defects have shown potential for creating single-photon emitters, which are valuable for applications in nano-optics and quantum technologies. Therefore, developing reliable, site-specific, and scalable methods for controlled defect creation is essential. He⁺-ion irradiation has been demonstrated as an effective technique for introducing precise point defects in TMDC lattices.(1) However, systematic and spatially resolved studies correlating He⁺-ion irradiation with optical modifications in TMDCs remain limited.

Here, we present a comprehensive study on the impact of He⁺-ion irradiation on the photoluminescence (PL) properties of mechanically exfoliated monolayer MoS₂ samples. We analysed the PL response from the He⁺-irradiated samples on SiO₂ across a range of doses: 10¹²-10¹⁵ ions/cm² and compared it against pristine samples. Our study shows a reduction in PL intensity from MoS₂ and a change in the relative intensity of A and B excitons with the increase of the irradiation dose. The deconvolution of PL spectra reveals that the ratio of B to A-exciton emission increases progressively with the irradiation doses before the PL emissions become fully quenched above an irradiation dose of ~10¹⁵ ions/cm². Relative increase in B-exciton's contribution is attributed to the increase in non-radiative processes caused by defects and charge impurities that are induced by He⁺-ion irradiation.(2) This is commensurate with the quenching of PL emission with increased doses along with the appearance of a defect emission band at a lower energy, which is further explored by conducting power-dependent PL spectroscopy. The role of substrate interaction on He⁺-ion irradiation has been investigated by conducting PL measurements on a suspended MoS₂ sample. Compared to supported samples, pristine suspended MoS₂ exhibits dominant neutral A-exciton emission with negligible B-exciton contribution. However, with increasing He⁺-ion doses, we observe a similar trend of B-exciton enhancement. The reduction in neutral excitons is accompanied by increased trion population and defect-related emission, attributed to charge doping and mid-gap states introduced by ion irradiation.

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UHV exfoliation of 2D materials

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2D materials are extremely 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. This allowed us to explore the properties of these materials in a pristine state. Here we will present our strategy, which provides pathway to reach this challenging goal.

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Localized Raman Spectroelectrochemistry in an All-Iron Aqueous Redox Flow Battery System

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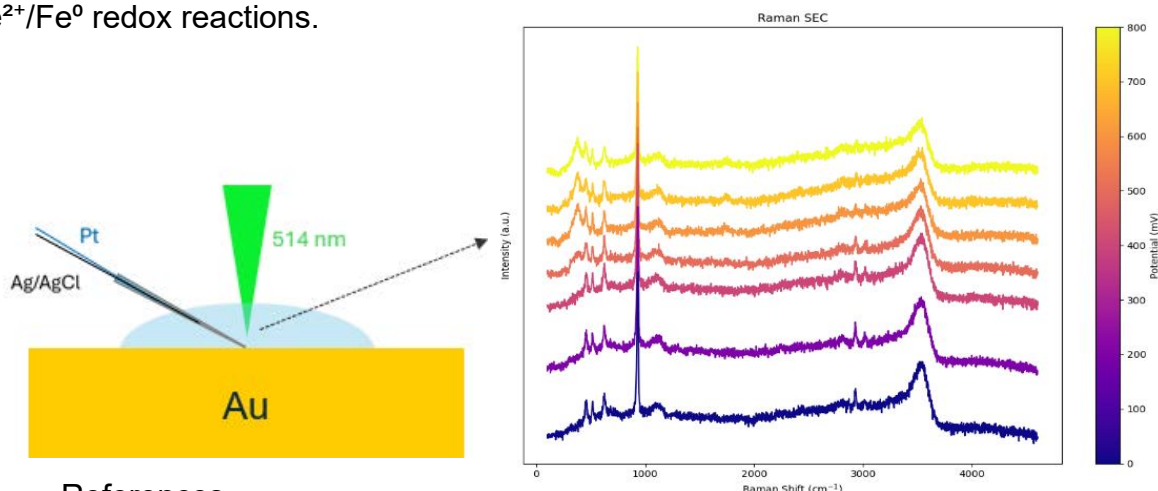
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Among large-scale energy storage technologies, redox-flow batteries (RFBs) stand out for their scalability and long cycle life [1]. While vanadium and zinc based RFBs are the most common, all-iron-based RFBs (AIRFBs) offer a cheaper and more environmentally friendly alternative without compromising safety.

To make iron plating/stripping in AIRFBs more efficient—that is, to suppress side reactions (such as HER) and dead metal growth while enhancing overall battery performance—it is necessary to optimize electrolyte additives [2].

The tested electrolyte consisted of $\text{Fe}(\text{ClO}_4)_3$, H_2O , and DMSO. Cyclic voltammetry measurements and in-situ spectroelectrochemical Raman experiments were conducted using a micro-droplet setup [3]. This approach allows direct observation of interfacial processes occurring at the outermost electrode surface, within the Helmholtz layer. A gold-sputtered working electrode provided surface signal enhancement. The system included a platinum counter electrode and an Ag/AgCl reference electrode. A 514 nm laser (~ 1 mW) was used to probe both $\text{Fe}^{3+}/\text{Fe}^{2+}$ and $\text{Fe}^{2+}/\text{Fe}^0$ redox reactions.



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LEEM Observation of Graphene Intercalation O₂, CO, H₂, H₂O and CO₂

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Since its discovery, graphene has attracted significant attention from the scientific community due to its unique properties. This interest has greatly expanded our understanding of two-dimensional materials. An interesting finding is that chemical reactions could be influenced (accelerated or modified) if occurring in the van der Waals space between graphene layer and a substrate [1]. For that, reactants must first intercalate beneath the graphene layer.

Although the concept of intercalation is straightforward, its practical realization is influenced by several factors, including the quality of the graphene, the choice of substrate, and the experimental conditions.

In this study, we investigate the intercalation of molecules beneath sub-monolayer graphene grown on a Pt(111) substrate (Figure 1). Platinum is selected due to its relevance as a catalytic material [2], while sub-monolayer graphene coverage is critical to initiate the intercalation process. Exposed regions of bare platinum allow incoming molecules to adsorb and dissociate, after which they can diffuse underneath the adjacent graphene flakes.

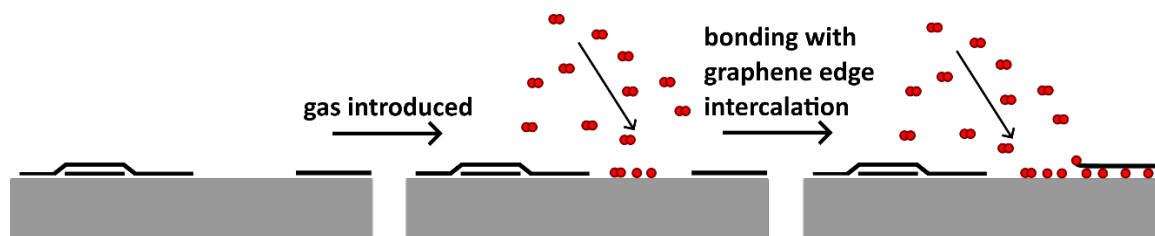


Figure 1: Scheme of intercalation of sub-monolayer graphene with multilayer areas.

As the second objective, we aimed to identify the most effective method for confirming the intercalation process. Typically, a range of characterization techniques, such as X-ray photoelectron spectroscopy (XPS), scanning tunneling microscopy (STM), and low-energy electron diffraction (LEED), are used for this purpose, although none gives bulletproof evidence of intercalation. In this study, a combination of low-energy electron microscopy (LEEM) and LEED proved to be particularly effective. Additionally, LEEM reflectivity measurements, commonly used for counting the layers of 2D materials [3], have been used to monitor the changes in graphene-substrate coupling and of the changes of van der Waals gap height.

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Raman spectroelectrochemical Insights into Doped Diamond Electrodes in Water-in-Salt Electrolytes

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Synthetic doped diamond is a promising electrode material due to its exceptionally high physical, chemical, and electrochemical stability, which can be utilized in various potential applications in electrochemistry, electrosynthesis, and energy storage systems. This study presents a comprehensive electrochemical and in situ Raman spectroelectrochemical (SEC) characterization of two types of boron-doped diamond (BDD) with *p*-type conductivity and phosphorus-doped diamond (PDD) with *n*-type conductivity in water-in-salt (WIS) electrolytes. We show that the doped diamond electrodes can achieve ultrawide electrochemical stability windows in highly concentrated and corrosive WIS electrolytes. While the performance of doped diamond materials has been extensively studied and documented in low-concentration electrolytes¹⁻³, their behavior in highly concentrated WIS electrolytes is less understood. Water and diluted aqueous electrolytes typically have narrow electrochemical stability windows (~1.23–2 V). This window can be significantly expanded by using highly concentrated WIS electrolytes with exceptionally high salt concentrations in combination with an appropriate electrode material⁴. The effects of boron and phosphorus doping levels, as well as the sp² carbon content, on the potential windows and the ensuing electrochemical stability, were examined in differently concentrated metal-perchlorate WIS electrolytes. Interestingly, the trends observed in WIS electrolytes differ from those observed in low-concentration electrolytes. Specifically, in WIS systems, as sp² carbon content increases, the potential stability window widens. In contrast, in low-concentration electrolytes, increasing sp² carbon content typically results in a narrower potential window⁵. The effects of BDD and PDD stability, as influenced by varying sp² carbon content and doping levels in both WIS and low-concentration electrolytes, are discussed based on electrochemical and in situ Raman SEC analysis.

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Optimising growth parameters for 2D transition-metal dichalcogenides using chemical vapour deposition

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The emergence of nanomaterials such as van der Waals heterostructures and atomically thin films/interfaces offers an exciting platform to explore reduced-dimensionality physics in the monolayer regime. Among them, semiconducting transition metal dichalcogenides (TMDs) stand out as a highly promising system for fundamental studies of two-dimensional (2D) materials, with potential applications in spintronics, optoelectronics, and valleytronics owing to their direct band gap in the monolayer limit and strong light-matter interaction. [1,2]

Despite over a decade of research on TMDs, achieving high-quality thin films through controlled synthesis remains a significant challenge in this field. Among the available methods, chemical vapour deposition (CVD) has emerged as a reliable approach to grow atomically thin layers. [3] The CVD growth is sensitive to several process parameters; in this work, we focus on varying temperatures and gas flow rates. Through systematic optimisation, the technique is refined to produce high-quality, wafer-scale thin films, yielding large-area monolayers and bilayers on SiO₂/Si substrate. Optical microscopy, Atomic force microscopy, Raman and Photoluminescence spectroscopy are employed to characterise the as-grown TMD films and validate these observations. [4]

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Wednesday, June 11

7:00-9:00	Breakfast		
9:00	Morning session:		
<i>Time</i>	<i>Chair</i>	<i>Speaker</i>	<i>Title of presentation</i>
9:00-9:40	J. Sambur	K. Bediako	Controlling interfacial electrochemistry with moiré superlattices
9:40-10:00		R. Kesarwani	Twisted Light-Matter Interactions: Advances, Challenges, and Future Prospects
10:00-10:20		V. Skákalová	Structure and properties of MoS ₂ and WS ₂ heterostructure synthesized in graphene oxide at ambient conditions
10:20-10:40		O. Volochanskyi	Graphene-templated Achiral Hybrid Perovskite: Unlocking Circularly Polarized light for Emission & Sensing
10:40	Coffee break		
<i>Time</i>	<i>Chair</i>	<i>Speaker</i>	<i>Title of presentation</i>
11:10-11:50	J. Kneipp	A. Grubišić-Čabo	ARPES studies of in situ exfoliated 2D materials using KISS method
11:50-12:10		J. Plšek	UHV exfoliation on the surface of reactive metals - MoS ₂ on Ti
12:10-12:30		N. Bendiab	Thermal Transport in Suspended Graphene
12:30	Lunch		
14:00	Departure to Telč (Castle tour and general sightseeing) / Departure for Roštejn		
17:45	Departure from Telč		
19:30	Conference dinner back in Třešť		

Controlling interfacial electrochemistry with moiré superlattices

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At electrode–electrolyte interfaces, crystallographic defects are frequently implicated as active sites that mediate interfacial electron transfer (ET) by introducing high densities of localized electronic states (DOS).¹ However, conventional defects are challenging to deterministically synthesize and control at an atomic level, hindering the direct study of how electronic localization impacts interfacial reactivity. Azimuthal misalignment of atomically thin layers produces moiré superlattices and alters the electronic band structure, in a manner that is systematically dependent on the interlayer twist angle.^{2,3} Using van der Waals nanofabrication of two-dimensional heterostructures, scanning electrochemical cell microscopy measurements, and four-dimensional scanning transmission electron microscopy, we report a strong twist angle dependence of heterogeneous charge transfer kinetics at twisted bilayer and trilayer graphene electrodes with the greatest enhancement observed near the ‘magic angles’.^{4,5,6} These effects are driven by the angle-dependent engineering of moiré flat bands that dictate the electron transfer processes with the solution-phase redox couple, and the structure of the relaxed moiré superlattice.^{7,8} Moiré superlattices therefore serve as an unparalleled platform for systematically interrogating and exploiting the dependence of interfacial ET on local electronic structure.

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Twisted Light-Matter Interactions: Advances, Challenges, and Future Prospects

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Twisted light, characterized by its orbital angular momentum (OAM), has opened new possibilities for controlling light-matter interactions in 2D materials, particularly monolayer transition metal dichalcogenides (M-TMDs). Over the past decade, experiments—including our own—have shown that OAM light can modulate excitonic populations, enhance valley polarization, and influence quasiparticle dynamics in van der Waals heterostructures. Increasing the topological charge of OAM light has been found to enhance exciton emission while suppressing trion formation, providing an optical handle to tune charge carrier densities without external doping or gating [1]. Twisted light has also been explored for optical trapping, quantum information processing, and structured excitonic transport in materials such as MoS₂, WS₂, and hBN-encapsulated heterostructures [2, 3].

While these studies provide valuable insights, many fundamental questions remain. Recent efforts suggest that OAM light could modify electronic band structures, spin-orbit interactions, and phonon-assisted transitions, but these effects remain largely unexplored in the context of strong light-matter coupling in 2D materials. Theoretical predictions of OAM-driven control of dark and bright excitons, nonlinear optical responses, and spin-charge momentum transfer require further experimental validation.

To address these challenges, we are developing an experimental setup at the Physics of Nanostructured group, Charles University, in collaboration with the Nanocarbon group, Heyrovský Institute, to investigate spin qubit control using twisted light. This system will operate at low temperatures (4 K) and high magnetic fields (0–14 T) to probe OAM-induced modifications in M-TMDs. Extending this research to room-temperature applications will help pave the way for next-generation quantum devices. A strong collaboration between experimental and theoretical efforts is essential to fully exploit twisted light for optoelectronics, valleytronics, and quantum computing.

Acknowledgements: The project “MSCA Fellowships CZ – UK3” (reg. n. CZ.02.01.01/00/22_010/0008220) is supported by the Programme Johannes Amos Comenius.

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Structure and properties of MoS₂ and WS₂ heterostructure synthesized in graphene oxide at ambient conditions

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In a previous work [1] we introduced a simple chemical synthesis of 2D metal iodides (2D-MI) embedded between graphene sheets where the desired 2D-MI is formed in graphene oxide at ambient conditions. Recently we succeeded to extend the method to synthesize 2D transition metal dichalcogenide, MoS₂ and WS₂, encapsulated in graphene. The chemical reaction also runs under ambient conditions. In this work, flakes of single-layer MoS₂ and WS₂ embedded between graphene sheets were widely characterised by Raman and electron energy loss spectroscopy, confirming presence of WS₂ or MoS₂ with reduced graphene oxide, whereas scanning transmission electron microscopy images show a dense appearance of single layer crystals of WS₂ or MoS₂ separated by graphene. The results of electrical conductivity measured in the temperature range from 4.2 up to 340 K indicate that the electronic transport is mediated through graphene flakes percolated network significantly doped by 2D crystals of MoS₂ and WS₂. We also measured negative magneto-resistance at low temperatures typical for weak localization mechanism in disordered systems.

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

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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 and without external magnetic fields. During the perovskite deposition, interactions at the graphene interface promote structural distortions, leading to local inversion symmetry breaking 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 spin-polarized photocurrent anisotropy factor (g_{ph}) up to ~ 0.51 , accompanied by a high photoresponsivity of $\sim 10^5$ 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.

ARPES studies of *in situ* exfoliated 2D materials using KISS method

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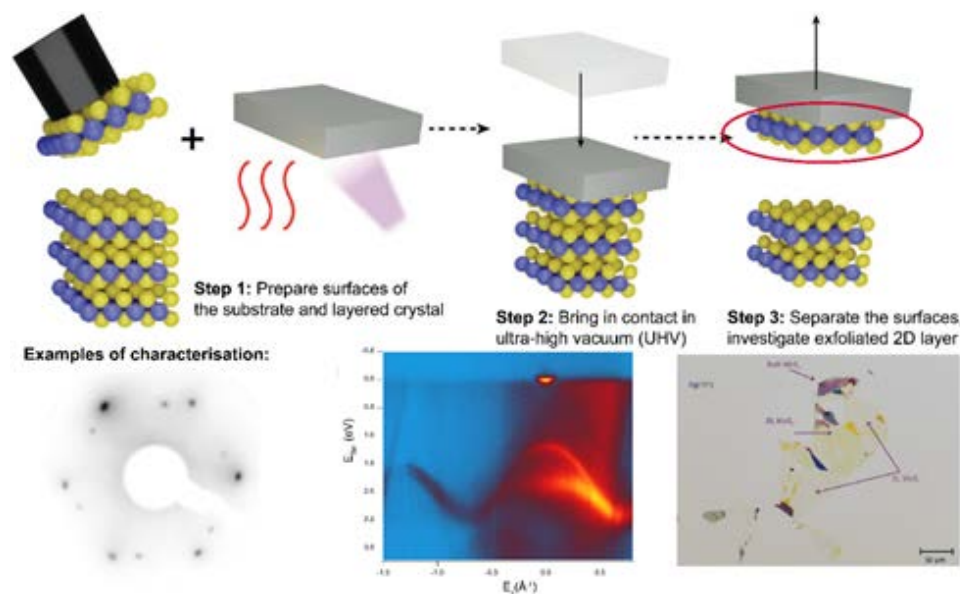
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Two-dimensional (2D) materials offer a rich platform for investigating novel quantum phenomena and designing nanostructures with tailored functionalities. However, key characterization techniques such as photoemission spectroscopy impose strict requirements on sample quality, size, and surface cleanliness — conditions that are often difficult to meet using standard mechanical exfoliation methods, even within a glove box environment.

In this talk, I will present a method for *in situ* exfoliation of 2D materials — the kinetic *in situ* single-layer synthesis (KISS) method — performed directly under ultra-high vacuum (UHV) conditions [1,2]. This technique enables the preparation of large-area, high-quality flakes with excellent crystallinity, and is particularly well-suited for air-sensitive materials, as it completely avoids exposure to ambient conditions.

Using the KISS method, we successfully exfoliated various semiconducting and metallic transition metal dichalcogenides, as well as kagome materials, onto Au, Ag, and Ge substrates, demonstrating the method's broad applicability. The electronic structure of these materials was subsequently probed using angle-resolved photoemission spectroscopy (ARPES), confirming the high quality of the KISS exfoliated samples.

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



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

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UHV exfoliation on the surface of reactive metals - MoS₂ on Ti

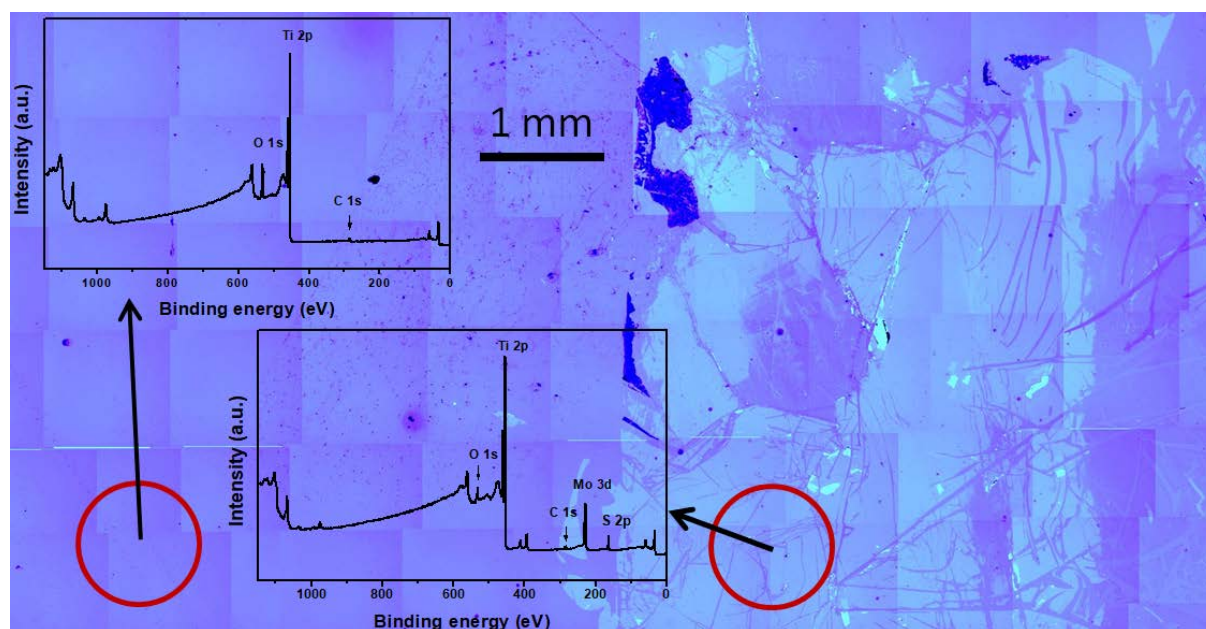
Jan Plšek^a, Abhilash Bajpai^a, Michele Gastaldo^a, Michaela Hanušová^{a,c}, Jan Honolka^b, Bazlul Karim^a, Luka Pirker^a, Václav Valeš^b, Martin Vondráček^b, Otakar Frank^a, Matěj Velický^a and Martin Kalbáč^a

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Metal-assisted exfoliation under ultra-high vacuum (UHV) conditions permits, besides high exfoliation yields [1] and the protection of sensitive 2D materials, the opportunity to study the interaction of 2D materials with clean and non-oxidized metal surfaces. In this work, we utilize fresh titanium layer as a substrate for exfoliating MoS₂ under UHV. Exfoliation of MoS₂ on Ti resulted in a centimeter-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. At the interface between the MoS₂ and Ti, we observed a polysulfide layer and the formation of TiS_x. Subsequently exposure of the sample to air led to oxidation of the metallic Mo and underlying Ti, disintegration of the polysulphides, and slight retrieval of MoS₂ content.



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Thermal Transport in Suspended Graphene

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Fourier law of heat transport seems to be no more applicable in 2D materials due to their extremely low thickness [1]. In particular, thermal physics of graphene is predicted to reach hydrodynamic to ballistic regimes of thermal transport [2,3].

Optothermal Raman spectroscopy has allowed estimating an effective thermal conductivity of graphene [4] and proven to be a promising technique for thermal measurements. However, so far, the extraction of the thermal coefficients from the actual measurements is not a direct procedure and the values reported in literature heavily depend on some assumptions in the models used.

Using two-laser Raman thermometry focused at the sub-micron length scale, we report static temperature maps and profiles of monolayer graphene suspended over a circular hole. We create a thermal distribution of phonons by heating the very center of the graphene membrane with a laser, while a second non-invasive laser records the frequency of the 2D active Raman mode over the surface. The signal is thereafter converted into spatial images of the local temperature field.

The obtained temperature profiles from the hot spot show an anomalous region surrounding the heated region that is interpreted using a non-local multi-linear extension of the Fourier law [7].

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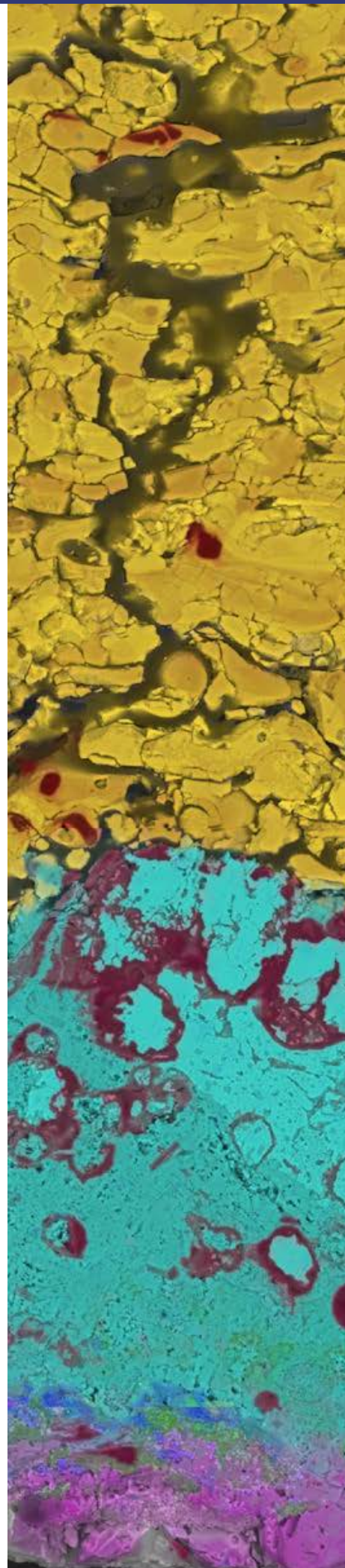
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- Live EDS Mapping
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- 3D rekonstrukce povrchu
- Analýza velikosti částic



Thursday, June 12

7:00-9:00	Breakfast		
9:00	Morning session:		
<i>Time</i>	<i>Chair</i>	<i>Speaker</i>	<i>Title of presentation</i>
9:00-9:40	R. Dryfe	J. Kneipp	Spectroscopy in the local fields of plasmonic structures for the characterization of bioorganic samples
9:40-10:00		R. Conan	Correlation of the Structural and Magnetic Morphology of Nanoparticles
10:00	Coffee break + check out		
<i>Time</i>	<i>Chair</i>	<i>Speaker</i>	<i>Title of presentation</i>
10:50-11:10	O. Frank	M. Gastaldo	Counting defects in monolayer MoS ₂
11:10-11:30		A. Bukhari	Defect-Engineered Two-Dimensional Materials: Towards a Holistic Perspective
11:30-11:50		A. Macková	Center of Accelerator and Nuclear Analytical Methods (CANAM) capabilities for 2D materials modification
11:50	Young Researcher Award Ceremony + Discussions Closure		
12:10	Lunch		
13:30	Departure for Prague		

Spectroscopy in the local fields of plasmonic structures for the characterization of bioorganic samples

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Vibrational (Raman and infrared) spectroscopy has become indispensable for our understanding of the structure and interaction of organic molecules in materials and biomolecular samples.[1] Surface enhanced Raman scattering (SERS) is not restricted to the well-known one-photon excited spontaneous Raman process that gives information on molecular composition, structure, and interaction through vibrational probing with high sensitivity. The enhancement mainly originates in high local fields, specifically those provided by localized surface plasmon resonances of metal nanostructures. High local fields can particularly support non-linear Raman scattering, as it depends on the involved fields to higher powers. By revealing plasmon-molecule interactions, non-linear Raman processes provide a very sensitive access to the properties of metal nanomaterials and their interfaces with molecules and other materials. The discussion will highlight the aspects of vibrational information that can be gained based on specific advantages of different incoherent Raman scattering and their surface enhancement. Apart from (field-enhanced) Raman scattering of known molecules, also their utilization in complex mixtures is within reach.[2] Possibilities to retrieve information from such data, and also their combination with nanoscale infrared experiments with such samples will be shown.

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Correlation of the Structural and Magnetic Morphology of Nanoparticles

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The design of magnetic nanoparticles (MNPs) relies on precise control of size, shape, and composition, as these parameters critically govern their performance in technological [1], biomedical [2], and environmental applications. A key challenge lies in resolving nanoscale magnetic morphology—including spin disorder and core-shell magnetization—since conventional techniques often lack sufficient spatial resolution. Polarized Small-Angle Neutron Scattering (SANS POL) overcomes this limitation by probing magnetization distributions at the nanoscale, enabling the disentanglement of spin disorder effects [3,4] and distinct core-shell contributions [5]. In this study, we investigate Mn-doped cobalt ferrite (CoFe_2O_4) nanoparticles synthesized via thermal decomposition, achieving uniform cubic shapes with narrow size distributions ($\sigma_{\log} < 10\%$). Using SANS POL, we correlate Mn doping levels with chemical homogeneity and magnetic structure, revealing tunable surface spin disorder. Furthermore, we evaluate the particles' hyperthermia performance under alternating magnetic fields, linking heating efficiency to their structural and magnetic properties. Our results provide a roadmap for optimizing doped ferrite MNPs, bridging fundamental insights with practical applications in biomedicine and beyond.

Acknowledgements

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Counting defects in monolayer MoS₂

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An important aspect of 2D materials is the number and type of defects in them. The most direct way to count defects is by using a microscopy technique with atomic resolution such as HRTEM or STM. However, these techniques are local and therefore very time consuming. In this aspect, Raman spectroscopy is a powerful tool for defect characterization. However, it relies on vibrational modes, making defect counting indirect and introducing significant uncertainty in the actual defect count. In our work, we combined Raman spectroscopy with scanning tunnelling microscopy to calibrate the defect counting in 2D materials. In particular, we studied exfoliated MoS₂ monolayers in which we created defects by He-ion bombardment. To exclude the effect of the substrate, we performed the ion bombardment both before (on the bulk MoS₂ crystal) and after the exfoliation on Au(111) substrates. This not only allows us to compare the effect of different substrates, but also to obtain a layer-by-layer depth profile of the number of defects in the bulk MoS₂ crystal.

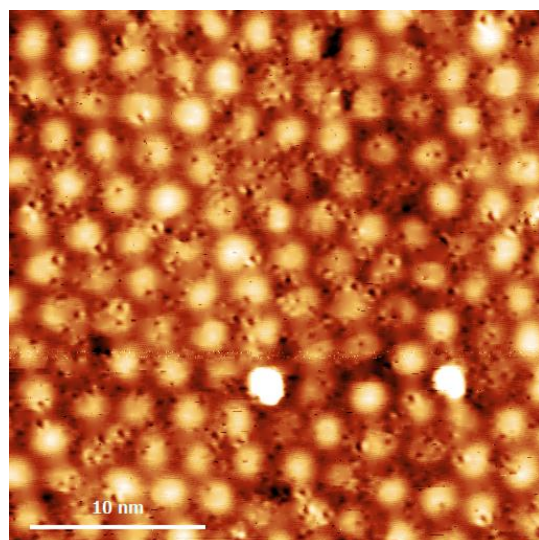


Figure 1. STM topography of a MoS₂ monolayer exfoliated on Au(111) after He⁺ bombardment.

Defect-Engineered Two-Dimensional Materials: *Towards a Holistic Perspective*

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Defects in two-dimensional materials (2DMs) have been studied for a number of years due to the potential applications that may stem from tuning their material properties. Various methods have been utilised to introduce the disorder, and their impact on the material's properties has been characterised with numerous techniques including optical spectroscopies, transport measurements and electron microscopies.^[1,2] However, a cohesive picture that ties together all of the physical regimes that underpin these properties, in terms of their dependence on the amount of disorder in the system, is still lacking. Our results here show how the evolution of the Raman and PL spectra of Molybdenum disulfide (MoS₂) can be contextualised in terms of its work function and other characterisations when defects are introduced through helium ion irradiation.^[3] Combining both micro- and nanoscopic techniques in this manner will provide a new perspective on the study of defects in 2DMs that may invigorate such studies to investigate materials beyond graphene and MoS₂.

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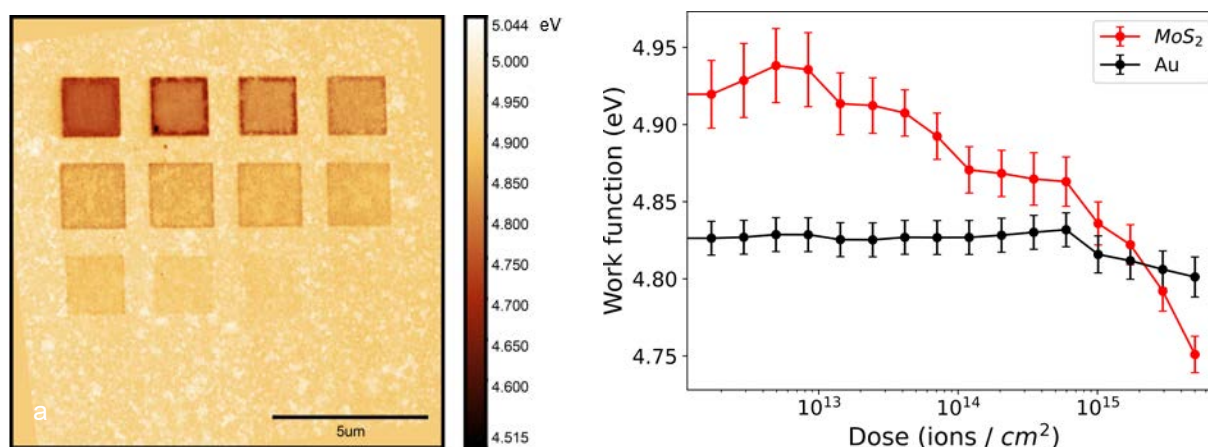


Figure 1: (a) – Work function map of monolayer MoS₂ obtained by Kelvin probe force microscopy. The increasing contrast of the squares indicates a greater defect density. (b) – Work function dependence on the helium ion dose used to create the defects in (a).

Center of Accelerator and Nuclear Analytical Methods (CANAM) capabilities for 2D materials modification

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The Centre of Accelerators and Nuclear Analytical Methods (CANAM), housed at the Nuclear Physics Institute (NPI) offers unparalleled capabilities that leverage beams of accelerated ions for a wide range of applications. These methods—dedicated to analysis, characterization, modification, and production—are crucial for addressing complex scientific challenges in physics, materials science, chemistry, biology, engineering, and environmental studies. Laboratory of Tandetron (LT) is producing ion beams with energies between 400 keV and 30 MeV for virtually all elements of the periodic table being an important part of CANAM. Tandetron accelerator enables precise investigations and material modifications through advanced techniques such as Rutherford Backscattering Spectrometry (RBS), Elastic Recoil Detection Analysis (ERDA), Particle-Induced X-ray Emission (PIXE), Particle-Induced Gamma-ray Emission (PIGE), and nanoscale imaging with an Ion Microprobe with submicron lateral resolution. These nuclear analytical methods allow material characterization, defect engineering, and nanoscale structuring—essential for applications ranging from nanooptics and electronics to bionics and wear-resistant materials. A focal point of LT research involves graphene and graphene-like materials, important for their remarkable carrier mobility, extensive surface area, two-dimensional architecture, and cost-effective nanoscale morphologies. These materials are proving invaluable in applications such as supercapacitors, ultrasensitive gas detectors, and energy storage devices. Graphene oxide (GO), a hydrophilic precursor to graphene, features functional groups like epoxides and hydroxyls that enhance its sensitivity to water molecules, making it particularly effective for sensors and catalytic applications.

Recent advancements in ion beam research at CANAM include:

- Ion Implantation of Metal Ions, such as copper, to enhance the photocatalytic activity of carbon-based materials like graphene oxide.
- Ion Lithography using microbeams to develop microdevices and tailor electronic structures with exceptional precision.
- High-Quality Microstructures, created through ion beam modification, enabling advanced technologies for pollutant degradation, energy storage, and sensor miniaturization.
- Functional Humidity Microsensors, developed using GO-based materials for precise environmental monitoring.

The research has been carried out at the CANAM (Centre of Accelerators and Nuclear Analytical Methods) infrastructure LM 2015056 and was supported by the Advanced Multiscale Materials for Key Enabling Technologies project, supported by the Ministry of Education, Youth, and Sports of the Czech Republic. Project No. CZ.02.01.01/00/22_008/0004558, Co-funded by the European Union.