J. Heyrovský Institute
of Physical Chemistry

CHARLES UNIVERSITY
Faculty of mathematics
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International Czech – Japanese Symposium on Advanced MultiScale Materials

In collaboration with:

Grant-in-Aid for Transformative Research Areas(A)
Science of 2.5 Dimensional Materials
Paradigm Shift of Materials Science Toward Future Social Innovation
2.5 D Materials

Book of Abstracts


26th - 28th September 2024
Prague, Czech Republic

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VENUE FOR THE CONFERENCE DINNER Thursday 26 September 2024 at 19:30

VILA LANNA

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Vítejte! - いらっしゃいませ！– Welcome!

Dear Colleagues and Honored Guests,

*It is a great pleasure to welcome you to the **Czech-Japanese Symposium on Advanced Multiscale Materials**. This gathering is a testament to the long-standing and fruitful scientific collaboration between the Czech Republic and Japan, two nations that share a deep commitment to innovation, research, and the advancement of technology.*

Our collaboration in science and technology has a rich history. One of the remarkable connections between our countries lies in the field of robotics. The Czech Republic gave the world the word "robot," introduced by writer Karel Čapek in 1920, while Japan has elevated robotics to an art form, becoming a global leader in perfecting robotic technologies and their applications. This symbolic link between our two nations highlights our shared contribution to the future of automation and advanced materials science.

We also recall the notable collaboration of Czech Nobel laureate Jaroslav Heyrovský, the inventor of polarography, with Japanese scientists, which paved the way for advancements in electrochemistry. This spirit of partnership continues today, as Czech and Japanese researchers work together on cutting-edge projects in materials science, nanotechnology, and beyond.

This symposium offers an invaluable opportunity for researchers and experts from both countries to exchange ideas, explore new frontiers in advanced materials research, and build on our existing collaborations. The progress will not only contribute to the scientific community but also have a profound impact on industry and society at large.

I extend my warmest wishes for a productive and inspiring symposium. May our discussions lay the foundation for future breakthroughs and strengthen the scientific bond between the Czech Republic and Japan.

Thank you, and I look forward to the exciting developments this collaboration will bring.

Jana K Vejpravova
Chair of the symposium

PROGRAM

Thursday 26.09.2024

9:00 - 12:15	***visit of MatFyz (UK)***	
12:30	Welcome	Profs. Vejpravova (MFF UK) & doc. Kalbac (HIPC CAS)
12:40	Plenary	**Prof. Ago**, Kyushu University: ***Large-Scale Growth and Integration of High-Quality 2D Materials for "Science of 2.5D Materials"***
13:15	Invited	**Prof. Miyata**, Department of Physics, Tokyo Metropolitan University: ***Growth, structures, and properties of transition metal chalcogenide nanostructures***
13:35	Invited	**Dr. Malínský**, ÚJF CAS: ***Ion beam micro-structuring of graphene allotropes for sensors***
13:55	Invited	**Prof. Sofer**, UCHT Prague: ***2D Materials from Xenes to novel 2D magnetic and dielectric materials***
14:15	Invited	**Prof. Matsumoto**, Tokyo Polytechnic University: ***Intercalations into graphite and multilayer and bilayer graphene using a vapor-phase method***
14:35	*Break*	
14:55	Invited	**Dr. Frank**, HIPC CAS: ***Impact of Defects on Mechanical and Electronic Properties of 2D Materials***
15:15	Invited	**Dr. Pu**, Tokyo Institute of Technology: ***Functional optoelectronic devices based on strained monolayers and heterostructures***
15:35	Invited	**Dr. Varade**, MFF UK: ***Proximity Effects in MoS_2 monolayer on Janus 2D magnet CrSBr***
15:55	Invited	**Prof. Machida**, Institute of Industrial Science, University of Tokyo: ***Symmetry engineering and subband electronics using van der Waals assembly of transition metal dichalcogenides***
16:15	*Break*	
16:35	Junior session (5 talks): R. Conan, S. Sahu, S. Nadupalli, H. Lyshchuk, S. Hricov	
17:15	***End of Day 1, tour Heyrovsky institute***	
19:30	***Conference Dinner at Vila Lanna***	

Friday 27.9.2024

9:30	Invited	**Dr. Červenka**, Institute of Physics CAS: ***Straintronics with 3D Cellular Graphene Aerogels***
9:50	Invited	**Prof. Nagashio**, The University of Tokyo: ***2D layered semiconductors: Challenge & Perspective***
10:10	Invited	**Prof. Yamada-Takamura**, Japan Advanced Institute of Science and Technology: ***Epitaxially-Stabilized Novel 2D Materials on Substrates***
10:30	Invited	**Dr. Cígler**, IOCB CAS: ***Designing Nanoparticles for Biological Environments***
10:50	Invited	**Dr. Zákutná**, Department of Inorganic Chemistry, Faculty of Science, Charles University: ***Magnetization distribution in core/shell magnetic nanoparticles***
11:10	*Break*	
11:20	Invited	**Prof. Takahashi**, Nagoya University: ***Real-space electrochemical imaging of catalytically active sites of two-dimensional materials***
11:40	Invited	**Dr. Klimeš**, Charles University: ***Testing the precision of pseudopotentials and related methods***
12:00	Invited	**Dr. Kočišek**, HIPC CAS: ***Ionizing Radiation and DNA-Based Digital Data Storage***
12:20	Invited	**Prof. Koshino**, Osaka University: ***Moiré Multilayers — Towards Topological Quasicrystals***
12:40	Invited	**Prof. Matsuda**, Institute of Advanced Energy, Kyoto University: ***Optical Physics and Quantum Science using Moiré Excitonic States in van der Waals Heterobilayer***
13:00	Closing	Profs. Kalbáč & Vejpravová

Saturday 28.9.2024

9:00 – 12:00	Round Table – free discussion

Large-Scale Growth and Integration of High-Quality 2D Materials for “Science of 2.5D Materials“

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Two-dimensional (2D) materials have attracted great interest because of their unique physical properties and various applications. The control of van der Waals (vdW) interaction and utilization of vdW nanospace are expected to extend the field of materials science, and such research direction can be expressed with a new concept of “Science of 2.5D materials”, as illustrated in Figure 1 [1,2].

In this presentation, our recent research is introduced based on this 2.5D concept. I will show our recent development of CVD growth of high-quality and large-area multilayer hBN, which can be used as a building block of various 2.5D materials, such as graphene field-effect transistors (FETs) [3]. The CVD-grown multilayer hBN improved the carrier mobility of monolayer graphene, especially when it is sandwiched with the hBN. In addition, few-layer hBN layers has been synthesized and applied to magnetic tunneling junction devices (MTJs), obtaining a high magnetoresistance (MR) ratio of ~10% [4].

I will also introduce our new result of the tape transfer of 2D materials, which is expected to accelerate the 2D/2.5D materials research and applications (Figure 2) [5]. We achieved clean and user-friendly transfer of graphene, MoS_2, WS_2, and hBN using the UV tapes whose adhesive force can be decreased about 1/10 by UV light illumination. We do not need to use organic solvent so that we can transfer them onto plastics, and the robust tape allows “cut-and-transfer” for site-selective transfer, which saves 2D materials and production cost.

Our recent result of the synthesis and applications of MoS_2 nanoribbons will be also introduced [6]. Dense and self-aligned MoS_2 nanoribbons grown by CVD showed high catalytic activity towards hydrogen evolution reaction (HER).

Finally, I will introduce our group research project named, “Science of 2.5 Dimensional Materials: Paradigm Shift of Materials Science Toward Future Social Innovation (Sept., 2021 to March, 2026)” which is supported by MEXT, Japan [7].

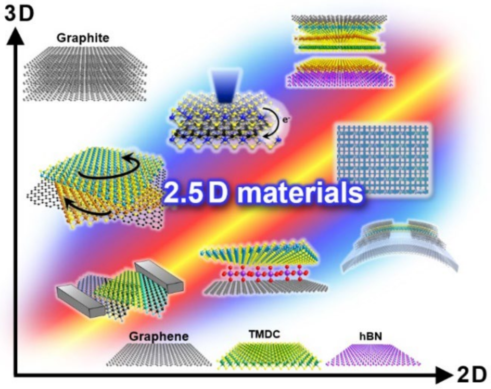

Figure 1: Concept of 2.5D materials [1,2].

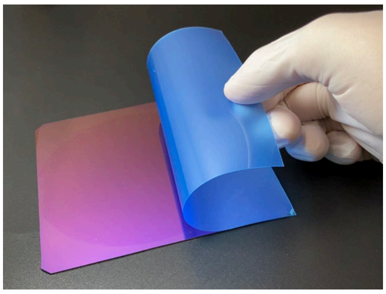

Figure 2: Tape transfer of 2D materials [5]. This photograph shows transfer of 4-inch monolayer graphene on a SiO_2 substrate [6].

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I-01

Growth, structures, and properties of transition metal chalcogenide nanostructures

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Transition metal chalcogenides (TMCs) are attractive materials with a wide variety of nanostructures and physical properties. Recent advances in growth techniques have enabled the preparation of various low-dimensional configurations of transition metal monochalcogenides (TMMs) and dichalcogenides (TMDs). In this talk, I will review on our recent progress in the fabrication and characterization of such nanostructures, including nanowires, nanotubes, nanoscrolls, nanoribbons, and in-plane/vertical heterostructures. For example, we have developed the controlled growth of TMD in-plane heterostructures with 1D interfaces [1-6]. These heterostructures have demonstrated functions such as the circularly-polarized and wavelength-tunable light-emitting diodes [2,3], directional exciton-energy transport [4], and tunneling field-effect transistors (TFETs) [5,6]. We have also used Janus TMDs to fabricate nanoscrolls and moiré superlattices. Built-in strain in Janus TMD monolayers allows the formation of nanoscrolls with small diameters [7]. The chalcogen substitution process can convert bilayer $MoSe_2$ into Janus $MoSSe/MoSe_2$ moiré superlattices by controlling the lattice constant [8]. Isolated boron nitride (BN) nanotubes have enabled the templated synthesis of single-wall TMD nanotubes [9,10]. In addition to TMDs, we have recently achieved the wafer-scale growth of atomically-thin TMM wires [11]. The bundles of TMM wires can be tailored into a thin, nanoribbon-like structure, where a 2D carrier gas is formed [12]. Such ribbon-shaped bundles have been further used for a conversion to layered TMD nanoribbons [13] and for synthesis of metal-intercalated ternary TMMs [14]. These developments pave the way for exploring the low-dimensional physics and potential applications of TMC nanostructures.

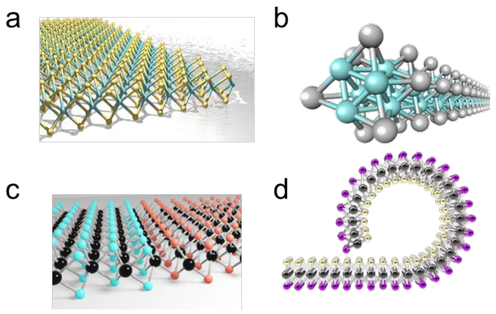

Figure 1. Examples of TMC-based nanostructures. (a) monolayer TMD, (b) TMM nanowires, (c) in-plane TMD heterostructures, and (d) Janus TMD nanoscroll.

References
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I-02

Ion beam micro-structuring of graphene allotropes for sensors

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The boom of miniaturized electronics has popularized research on microscale devices, such as microsensors for health monitoring. Organic solids based on graphene derivatives, especially graphene oxide (GO), are excellent candidates for the fabrication of chemo-resistive sensors due to their ability to detect at room temperature, excellent sensitivity, mechanical stability, short reaction time, low cost, commercial availability, easy processing, and flexibility. Furthermore, doping the GO with metals or metal oxides leads to a further improvement of its sensory properties. Ion-beam lithography is a highly localized and precise technique for modifying chemical and functional properties (patterning), which, in the case of organic compounds, allows for tailoring the desired properties (degree of reduction, modification of sp^2/sp^3 ratio of carbon hybridization, sensory/catalytic properties, and dielectric properties). Additionally, ion irradiation has several advantages, such as the absence of chemical agents, the absence of unwanted oxide formation, less formation of residual impurities, and potentially scalable and cost-competitive production. Unfortunately, direct ion-beam lithography (without a mask) with heavy metal ions remains a challenge due to the difficulty of focusing a MeV heavy ion beam into a micrometer-size spot. This promotes the dominance of mask-based ion beam lithography to micropattern the material with heavy ions.

For this reason, we attempted to prepare micro-scale capacitor-like structures (900x900 µm) in graphene oxide (GO) using energetic carbon and copper ion beams in two ways. One approach involved ion beam writing, while the second utilized ion beam implantation through a polymeric mask. The polymeric mask was prepared directly on the surface of the substrates by spin coating of PMMA, followed by proton beam writing and development in isopropyl alcohol. After the ion beam implantation, the mask was removed using acetone. The GO foils were irradiated by 2.5-5 MeV ion beams with an ion fluence of 1800 and 3600 $nC.mm^{-2}$. Subsequently, the shape of the created micro-structures and compositional changes of the irradiated materials were studied using Scanning Electron Microscopy (SEM)/Energy-Dispersive X-ray spectroscopy (EDS) methods, respectively. Complementary structure and compositional changes in the irradiated area were characterized by micro-Raman spectroscopy, X-ray Photoelectron Spectroscopy (XPS), Rutherford Back-scattering Spectroscopy (RBS), and Elastic Recoil Detection Analysis (ERDA) spectroscopy. The irradiation of non-conductive materials leads to deoxygenation, carbonization, and creation of new carbon bonds, resulting in increased electrical conductivity. The electrical and humidity sensing properties of the prepared microstructures were also tested and compared to the commercial sensor Bosch BME2820 and to each other. We can conclude that the structures prepared by carbon implantation through the PMMA mask show very similar properties to those prepared by carbon microbeam writing.

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I-03

2D Materials from Xenes to novel 2D magnetic and dielectric materials

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The recent progress in methods of high quality and low defect 2D magnetic materials will be discussed. Beside the group of transition metal halides and chalcogens also the rapidly growth family of mixed halogen-chalcogenides will be introduced. The dominantly explored material, chromium sulfo-bromide adopt FeOCl structure and possess A type antiferromagnetic ordering at low temperature. By various methods of exfoliation or defect formation, this material can be converted to ferromagnetic state. The chemistry of CrSBr including doping and possible covalent and non-covalent functionalization and its effect on magnetic and optical properties will be presented together with possible applications in electronic devices. Beside the two dimensional magnets, the 2D dielectric exhibit important group of materials with crucial rule in device fabrication. The broad spectra of novel high-k 2D dielectric materials growth and applications will be presented together with large scale crystal growth of hexagonal boron nitride at atmospheric pressure using various metal flux.

I-04

Intercalations into Graphite and Multilayer and Bilayer Graphene using a Vapor-phase method

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Graphite can intercalate various chemical species, leading to the formation of graphite intercalation compounds (GICs). GICs have been studied extensively for almost a century. In addition to graphite, bilayer and multilayer graphene are widely used to produce intercalated graphene compounds. Numerous studies have focused on investigating the intercalated forms of graphene. Intercalation plays an important role in controlling specific properties of graphite, particularly its electrical properties. This indicates that the intercalation technique can potentially be used in various graphene applications. We are currently investigating intercalation of graphene and similar materials using a vapor-phase method that produces isolated, pure intercalation compounds. In this study, we found that most of the intercalated species for graphite are also capable of intercalating into graphene; however, the reverse is not true. Thus, graphene appears to be more suitable than bulk graphite as an intercalation host material. I am currently exploring intercalations of graphene and similar materials.

One of the two-dimensional materials we have studied is graphene-like graphite (GLG). GLG is a material very similar to graphite, but contains oxygen and many defects, with interlayer distances greater than those of graphite. We found that GLG is easier to intercalate than graphite. Figure 1 shows the XRD patterns and Raman spectra for the intercalated products of GLG. Although Na is difficult to intercalate in graphite, stage 1 compounds were formed with GLG. Similarly, while Mg doesn't intercalate into graphite, the stage 1 peak appeared in the XRD pattern when GLG was used.

In this presentation, we introduce various intercalated compounds whose hosts include graphite, multilayer and bilayer graphene, and other similar two-dimensional materials.

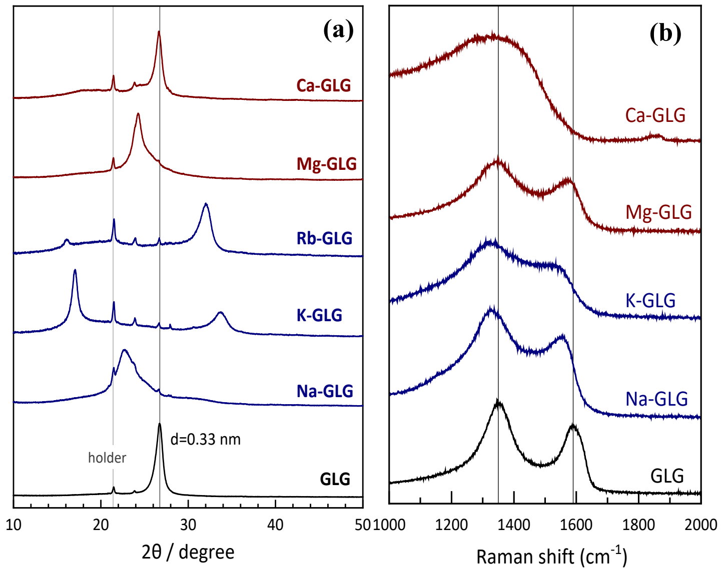

Fig.1 XRD patterns (a) and Raman spectra (b) for products of GLG.

Acknowledge
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I-05

Impact of Defects on Mechanical and Electronic Properties of 2D Materials

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Defects are ubiquitous in any crystalline material, the 2D materials being no exception. There are many different kinds of structural defects and their presence can be both advantageous and adverse, depending on the particular application. In 2D materials, all defects will impact the properties at scales ranging from nano- to macro-, as they are both in the material's "interior" and at the surface at the same time. Therefore, it is essential to control their formation and spatial distribution, and to study the influence each type of defect has on the local and global behavior of the material.

The role of defects induced by oxygen plasma and ion irradiation will be discussed in relation to, e.g., contact resistance of 2D materials, charge-transfer processes at the interface between the 2D material and an electrolyte [1], and mechanical properties [2]. Special emphasis will be given to highlighting the advantages of using in-situ Raman spectroscopy in both mentioned cases. In [1], the utilization of localized in-situ Raman spectroscopy within a microdroplet electrochemical cell enables to address only the basal-plane defects and not the edge-defects, which commonly obscure the effects of the basal-plane ones. In [2], in-situ Raman spectroscopy is essential for providing an independent method able to quantify the real strain attained in graphene during force-distance measurements.

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I-06

Functional optoelectronic devices based on strained monolayers and heterostructures

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Atomically thin transition metal dichalcogenides (TMDCs) and their heterostructures are attractive for functional optoelectronic applications because of their diverse bandgaps and band offsets, robust exitonic emission and absorption, and unique quantum (spin-valley) properties [1]. In particular, recent demonstrations of symmetry control/engineering in TMDCs provide an interesting approach to invoke new optoelectronic functionalities such as bulk photovoltaic effects [2]. Here, to directly control the crystal structure/symmetry of TMDCs, we focus on the strain effects because of excellent mechanical flexibility of monolayers. We can directly modulate band structures and band alignments in TMDCs and their heterostructures by the strain-induced lattice structure/symmetry modulation, which yields distinctive device functionalities, including in anomalous photovoltaic effects, robust chiral light emission, and wide-range optical modulation [3-6].

In this talk, we mainly focus on three functional devices which utilize the strain effects. First one is the room-temperature electrical tunable chiral light-emitting devices using strained monolayer TMDCs (Fig. 1, top) [3]. We can effectively control circularly polarized light emission by strain-induced band structure evolution. Second is the in-plane heterostructure devices, which also create room-temperature chiral light emission via strain effects at junction interfaces (Fig. 1, middle) [4]. Third is the alloy devices with composition gradient (Fig.1, bottom). We can realize continuous color-tunable light emission and anomalous photovoltaic effects accordingly to the spatial composition distribution [5,6]. Moreover, we also introduce recent advances of direct control of Moiré pattern in TMDC heterostructures by strain effects. Unusual Moiré pattern such as rectangle- and 1D-like pattern can be accordingly modulated by continuous strain tuning.

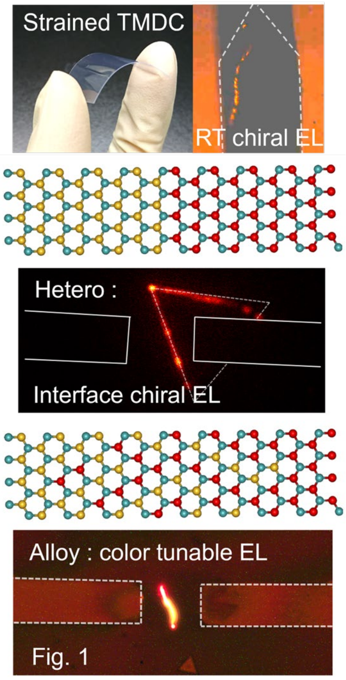

Fig. 1

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I-07

Proximity Effects in MoS_2 monolayer on Janus 2D magnet CrSBr

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Heterostructure engineering and the study of 2D magnets are at the forefront of contemporary materials science, offering unique opportunities to explore novel physical phenomena. In this study, we investigate the intriguing properties of a heterostructure composed of a MoS_2 monolayer exfoliated onto a few layers of 2D Janus magnet CrSBr. Using cryogenic magnetic circularly polarized Raman and photoluminescence (PL) and time-resolved (TR) PL measurements, we explore the proximity-induced spin-phonon coupling and valley polarization.

Our Raman measurements reveal that both the A_1' and E'Raman modes of MoS_2 are influenced by the magnetic ordering of CrSBr, showing a blue shift as the temperature decreases. This shift saturates around the Néel temperature of approximately 140 K, indicating proximity induced strong spin-phonon coupling.

Proximity effects are further evidenced by the dependence of the exciton-to-trion ratio in MoS_2 on the magnetic ordering of CrSBr, with a notable transition observed near the Néel temperature. The degree of circular polarization (DCP), a crucial parameter for measuring proximity effects (Nature Nanotechnology, **15**, 2020, 187), shows that the exciton and trion DCP curves follow the magnetization curve of, with a saturation field around 1.8 T at 10 K (Nature Commn. **13**, 2022, 4745). Analyzing the valley Zeeman effect, we find an exciton g-factor of approximately 4.4, slightly enhanced compared to the pristine MoS_2, while the trion g-factor is anomalously high at around 66.6. This significant enhancement can be attributed to the strong proximity effects. The local magnetic field from CrSBr interact with charged trions in MoS_2, causing additional spin splitting in trions due to proximity effects. Magnetic exchange interactions between CrSBr's magnetic moments and MoS_2 trions significantly modify the trion energy levels. Additionally, the field-dependent PL peak of CrSBr around 1.73 eV can influence trion emission in MoS_2, highlighting the dynamic interaction and importance of magnetic fields in modulating the heterostructure's electronic properties. Further, the temperature and magnetic field dependence of exciton life is estimated using TRPL to distinguish proximity effect on MoS_2.

Additionally, we observe that the PL enhancement of MoS_2 can be modulated by the thickness of CrSBr. This modulation is attributed to the n- to p-type doping transition of 1L-MoS_2 upon contact with CrSBr, resulting from the type-II band alignment, which fundamentally alters the electronic properties of the heterostructure.

Our findings demonstrate strong proximity effects in MoS_2/CrSBr heterostructures, offering new avenues for exploring novel physics as well as paving the way for innovative technologies in the realm of photo-spintronics and logic device functionalities. The integration of excitonic and magnetic material heterostructures into devices could lead to advancements in tunable photonic elements, development of magneto-optical devices, and novelties in spin-based quantum information processing, highlighting their potential in next-generation technological applications.

I-08

Symmetry engineering and subband electronics using van der Waals assembly of transition metal dichalcogenides

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The most distinct feature of van der Waals (vdW) junctions of 2D materials is controllability of twist angle between the crystals, which modulates the band structure and material properties. Here, we demonstrate that the spatial inversion symmetry and hence the spin splitting in band structure can be controlled by vdW assembly. Twisted bilayer WTe_2 with twist angle $\theta_{\text{twist}} = 0°$ and 180° are investigated. The intensity of second harmonic generation changes by two orders of magnitude depending on θ_{twist}, indicating that 1L WTe_2 +1L WTe_2 (0°) possesses the spatial inversion symmetry, whereas 1L WTe_2 +1L WTe_2 (180°) lacks the inversion symmetry. The electronic structure of the 1L WTe_2 +1L WTe_2 are significantly modulated by θ_{twist}. The spin splitting emerges when $\theta_{\text{twist}} = 180°$ due to the broken inversion symmetry.

Few-layer transition metal dichalcogenides (TMDs) exhibit subband quantization induced by the out-of-plane quantum confinement of the wavefunctions, i.e., a few-layer TMDs is a naturally-formed quantum well (QW). Using momentum-conserved resonant tunneling, we investigate the QW states in 4L-WSe_2/h-BN/4L-WSe_2 vdW tunnel junctions with tunnel twist angles θ_{tunnel}. Current–voltage characteristics exhibit multiple resonant tunneling peaks whose positions shift as θ_{tunnel} was varied over the 0–60° range, which indicated the presence of a spin-polarized subband crossing and a saddle point. Our twist-controlled resonant tunneling approach overcomes the difficulties associated with momentum-resolved electronic structure measurements and reveals the unique vdW-QW states in the conduction band of multi-layer WSe_2.

Finally, we demonstrate 3D manipulation technique of 2D material flakes, such as sliding, rotating, and folding. A PVC/PDMS micro-dome structure functions as a point-of-contact manipulator for 2D material flakes. The adhesion between the PVC polymer and 2D material is tunable with temperature. Our method could facilitate the expansion of vdW heterostructure fabrication technology for constructing more complex vdW structures.

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JUNIOR SESSION

Correlation of the Structural and Magnetic Morphology of Nanoparticles

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Magnetic nanoparticles (NPs) are of extraordinary interest due to their application in technology (data storage, spintronics) [1] and biomedicine (hyperthermia, drug delivery) [2], and that's thanks to their peculiar properties, such as superparamagnetism. Understanding how the macroscopic characteristics of MNPs and their ensembles connect to their structural and magnetic properties is critical to achieve top performance in a specific application. Despite the widespread interest in MNPs, the magnetic morphology and spin structure present significant challenges due to the limitations of traditional macroscopic techniques. However, the magnetic small-angle neutron scattering technique with incident beam polarization (SANSPOL) is a powerful tool for examining magnetization distribution at the nanometer scale, unravelling the impact of the spin disorder [3, 4] or magnetization from the core and shell parts of core-shell nanoparticles [5].

In this study, we aim to demonstrate how the chemical composition influences the magnetic structure of manganese (Mn)-doped ferrite MNPs. Using the thermal decomposition method, we have achieved distinct doping concentrations by precisely controlling the varying Mn doping levels in cubically shaped $CoFe_2O_4$ NPs of uniform particle size with narrow size distribution ($\sigma_{log} < 10$ %). Employing SANSPOL experiments, we have examined the chemical consistency and magnetic configuration of the resultant NPs, highlighting the correlation between surface spin disorder and the chemical composition of nanoparticles.

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JUNIOR SESSION

Optical behavior of CrSBr and its heterostructures with TMDCs

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In this talk, I will discuss the unique properties and applications of van der Waals materials, focusing on CrSBr and its interactions with monolayer (1L) transition metal dichalcogenides. CrSBr, an air-stable magnetic semiconductor, exhibits intriguing features like crystalline anisotropy and layer-dependent antiferromagnetism. We investigate its Raman properties, particularly in the anti-Stokes regime, revealing a high anti-Stokes to Stokes ratio at room temperature. Additionally, we examine the photoluminescence (PL) of 1L-MoS_2 when integrated with CrSBr in van der Waals heterostructures. Unlike typical quenching in PL due to nonradiative recombination, CrSBr layers up to 18 nm enhance the PL of 1L-MoS_2, while thicker layers cause quenching. This enhancement is due to n- to p- doping transition in 1L-MoS_2 upon contact with CrSBr, confirmed by Kelvin probe force microscopy and transport measurements. These findings highlight new strategies for optimizing PL in TMDCs and advancing next-generation optoelectronic devices.

Topological ferromagnetism in low-dimensional $BiFeO_3$ - Possible/impossible?

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The coupling between the electric and magnetic ordering in $BiFeO_3$ (BFO) (structure with displacements and tilts depicted in Figure a) is mediated by a spin orbit (see cartoon in Figure b) based on the Dzyaloshinskii-Moriya (DM) interaction (depicted in Figure c). DM phenomenon describes the interaction between neighboring ions in the crystal, that arise through partial electron transfer from the Fe^{3+} to neighboring O^{2-} ions.[1-3]

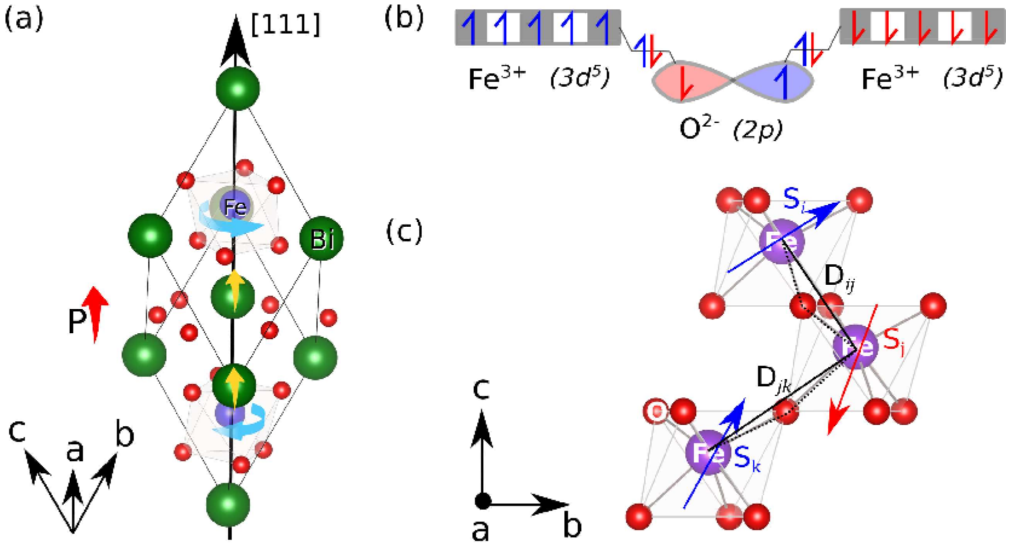

Figure 1: (a) Structure of BFO (b) Spin-orbit interaction and, (c) DM interaction

Recently, researchers discovered that the “skin” layer (top 5 nm) of BFO is under 0.7% strain, which results in an elongated out-of-plane lattice parameter and exhibits a unique electronic structure different from that of bulk rendering it ferro electrically/elastically dead. Additionally, theoretical investigations indicate the presence of microscopic elastic effects due to mono and di vacancies.[4]

The reports on skin layers and their disorder suggest a possibility of detecting topological ferromagnetism when the thickness of BFO film is lower than its period of the spin cycloid. Furthermore, the topological spin distortion due to the skin layer might compete with the spin-exchange phenomenon in doped BFO. Such phenomena points towards a milestone, meaning, it could significantly reduce the voltage required to switch the spin in BFO, potentially achieving an attojoule switching device.[5-6] This talk will present a brief overview of the above hypothesis along with a design of experiments.

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Electron-induced ligand release of the FEBID precursor

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This study aims to understand the chemical reactions fundamental to the dissociative ionization of trimethyl(methylcyclopentadienyl)platinum(IV) ($MeCpPtMe_3$), a common precursor of platinum in nanofabrication using focused electron beam. Previous studies probing the electron-driven chemistry of this precursor with surface-science techniques [1, 2] revealed a surprising phenomenon: the primary product released upon electron irradiation is not the methyl radical but rather the methane molecule. The gas-phase study by Engman et al. [3] provided a wealth of interesting data but did not address this specific question.

In the present work, gas-phase $MeCpPtMe_3$ was irradiated with electrons of controlled energy, and the positive product ions were analyzed using a reflectron time-of-flight mass spectrometer (RTOF). By studying the electron-impact dissociative ionization of $MeCpPtMe_3$ under single-collision conditions, we found that the removal of two methyl radicals is energetically more favorable than the removal of one radical and even energetically comparable to the non-dissociative ionization of $MeCpPtMe_3$. Quantum chemical calculations suggest that this effect can be explained by the rearrangement of the $MeCpPtMe_3^+$ ion prior to dissociation, resulting in the removal of ethane instead of two methyl groups.

This fragmentation pathway is computationally confirmed by irradiation-driven molecular dynamics (IDMD) simulations using the advanced software package MBN Explorer [4]. The results of the simulations are in good agreement with experimental data and pave the way for the widespread application of this approach to the description of radiation-induced chemical transformations in various molecular systems.

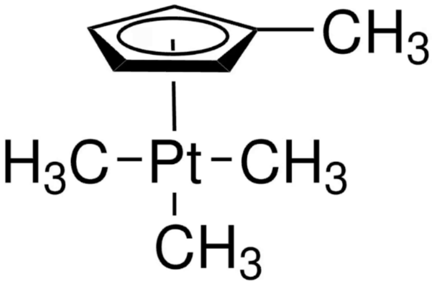

Figure 1: Trimethyl(methylcyclopentadienyl)platinum(IV) ($MeCpPtMe_3$)

Acknowledgments
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Magnetic morphology of a ε-Fe$_3$N multishell nanoparticles

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Many efforts have been made to investigate nanoscale magnetism showcased by magnetic nanoparticles (MNPs). The reasoning for such intensive research must be sought in the proposed applications of MNPs. Within biomedicine, one can point out a possibility of utilizing the MNPs as a contrast agent in diagnostical imaging or as a novel anti-cancer agent, where heat release via hyperthermia is suggested [1]. A typical example of nanomaterial with such applicability is iron oxide MNPs. However, in this work, we are proposing an alternative, the ε-Fe$_3$N. In its bulk form, it outperforms the iron oxides. Thus, we present you with a thorough investigation of a passivated ε-Fe$_3$N MNPs, aiming to disentangle its magnetic properties. The mean particle diameter was 17.2(2) nm, and the core@shell morphology was observed. Nevertheless, while comparing the bulk saturation magnetization with the magnetization measurement, we uncovered low saturation magnetization ($M_S \approx 40$ emu/mg) [2]. Thus, the volume-weighted, macroscopic measurements turned out to provide an incomplete picture of the passivated ε-Fe$_3$N MNPs' magnetic nature. Instead, we needed to examine the MNPs at the microscopic scale. To achieve this, small-angle neutron scattering experiments with incident beam polarization and the applied magnetic field were performed on the D33 instrument at ILL [3]. As a conclusion of our research, we unveiled the magnetic nature of ε-Fe$_3$N MNPs with a detailed description of MNP's core and shell magnetizations.

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Straintronics with 3D Cellular Graphene Aerogels

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Graphene, a two-dimensional (2D) carbon variant, has emerged as one of the most researched materials due to its remarkable electronic, thermal, mechanical, and chemical properties. These intriguing properties give it significant potential as a novel molecular building block for creating large-scale three-dimensional monoliths. In this work, it is shown that free-standing 3D graphene aerogels made of covalently cross-linked graphene sheets can demonstrate very different properties compared to 2D graphene. Graphene aerogels have ultra-low density, large specific surface area, and adjustable pore size. While 2D graphene is the best thermal conductor, 3D graphene aerogel exhibits the lowest thermal conductivity but very high electrical conductivity [1]. Moreover, 3D graphene exhibits exceptional elasticity, fire-retardant, and self-extinguishing properties [2,3]. Free-standing graphene layers assembled into a 3D cellular structure have 1000 °C higher flame resistance than 2D graphene on a substrate [2]. The cellular graphene aerogels resist flames at a temperature of 1500 °C for a minute without degrading their structure or properties. 3D graphene aerogels also feature innovative functions in energy storage, tactile sensors [4], and terahertz (THz) applications [5]. 3D graphene aerogels, unlike 2D graphene, exhibit high absorption over a broad range of THz frequencies, which can be modulated by strain, enabling dynamic THz modulation [5]. The graphene aerogel modulator can be tuned to exhibit either shielding capability or stealth characteristics. These findings open new avenues for leveraging 2D materials in their 3D porous form, where strain-induced changes in interlayer interactions enable unique control over the properties of these materials.

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I-010

2D layered semiconductors: Challenge & Perspective

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This talk will present the present status and future perspective of 2D layered semiconductors based on the advantage of 2D systems. The distinct advantages are their ultrathin nature and lack of dangling bonds. These properties are suitable for ultra-short channel FETs with ideal interface properties [1] because of the gate controllability. Moreover, tunneling FET with SS < 60 mV/dec is also demonstrated because superior interface properties prevent from generation current at the heterointerface [2], which is difficult to be achieved with the conventional semiconductors. As one of other electron devices, ultrafast Flash memory operation of 50 ns is successfully achieved because of extremely high dielectric breakdown field of *h*-BN under short voltage pulses [3]. I will also describe the current injection into *h*-BN for power device applications [4]. If times allow, unique optical device using bulk photovoltaic effect will be introduced [5]. Through these studies, fundamental advantages and limits are discussed for future development.

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I-011

Epitaxially-Stabilized Novel 2D Materials on Substrates

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One way to realize novel two-dimensional (2D) materials which lack “layered host materials” is to grow them epitaxially on single-crystalline substrates. Such materials must be characterized by complementary methods, and first-principles calculation is necessary to understand their crystal and electronic structures. Our group has been working on a variety of such materials by collaborating with other groups in the world.

“Silicene” is a Si-version graphene, having a buckled honeycomb structure. We have demonstrated, in 2012, by a combination of scanning tunnelling spectroscopy (STM), core-level and angle-resolved photoelectron spectroscopy (ARPES), and first-principles electronic structure calculations, that on epitaxial ZrB_2(0001) films grown on Si(111) substrates, Si atoms segregate to the film surface and crystallize in a honeycomb structure having stripe domains [1,2]. Although this silicene sheet is reactive against oxygen in air, it can be protected by “white graphene”. Through nitridation of ZrB_2(0001) film surface in ultrahigh vacuum, it is possible to form a hBN monolayer on film surface, and by exposing this surface to Si vapor, Si atoms intercalate in between hBN monolayer and ZrB_2(0001) film surface forming silicene protected by an insulating atom-thick layer [3].

When the substrate of ZrB_2(0001) film growth is changed to Ge(111) wafer, we found that a 2D Ge lattice having a “bitriangular” structure form instead of germanene. We have grown epitaxial, single-crystalline ZrB_2(0001) thin films on Ge(111) substrates, and by combing STM, total reflection high energy positron diffraction, photoelectron spectroscopy, and first-principles calculations, we found that Ge atoms segregate and crystallize into a bitriangular structure on the ZrB_2 film surface [4]. Our theoretical study on freestanding bitriangular lattice demonstrated that the flat band of a kagome lattice can be embedded in this very different structure [5]. The electronic structure measured by ARPES reveals “nearly” flat band at room temperature.

We have also found a new polymorph of monolayer GaSe when GaSe thin film is grown on Ge(111) substrate. Bulk GaSe is a semiconducting monochalcogenide and is known to crystallize in four “polytypes” which differ in how layers are stacked via van der Waals interaction, but no “polymorph” has been reported based on experimental study, including other layered monochalcogenides with the same crystal structure, such as GaS and InSe. Through detailed cross-sectional scanning transmission electron microscopy of GaSe thin films grown on Ge(111) substrates, we found that monolayer GaSe with “trigonal anti-prismatic structure”, which is a new polymorph, exist near the film-substrate interface [6]. Our first-principles study implies that the new phase is a metastable phase and can be stabilized under tensile strain [7].

All these new 2D materials were stabilized on substrates, and were recognized for the first time through our careful investigations.

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I-012

Designing Nanoparticles for Biological Environments

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The use of nanoparticles in diagnostics, therapeutics and imaging has revolutionized these fields with new properties not available with small molecules. Nanoparticle interface provide possibilities for polyvalent and independent attachment of different molecules serving as recognition/targeting structures, optical probes, spin probes or catalysts. However, nanoparticles operating in biological environments require precise control of multiple factors related to surface chemistry and their composition. To avoid for example aggregation, off-target interactions, and protein corona formation, appropriate interface design is essential. This talk will present general nanoparticle design strategies and specific examples including nanodiamonds and lipid nanoparticles.

I-013

Magnetization distribution in core/shell magnetic nanoparticles

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Tailoring magnetic nanoparticles (NPs) by choosing a suitable combination of size, shape, and material is the basis for realizing various technological (data storage, spintronics)[1], biomedical (magnetic hyperthermia, drug delivery)[2], or environmental applications. Success in designing systems to fulfill these applications requires a fine tune in the magnetic properties of the NPs, which is directly related to the control of the composition and morphology of the system[3,4]. In particular, the development of fabrication techniques of systems with complex architecture, such as core/shell or even onion-like multiphase NPs, gives new degrees of freedom to tune specific physical-chemical properties by combining materials with different compositions and magnetic characteristics and providing new perspectives for their potential applications. Despite the significant fundamental interest and technological importance of core/shell NPs, the magnetic morphology and spin structure are the key challenges to resolve, which are not accessible by conventional macroscopic techniques.

However, the characterization with traditional and affordable techniques is challenging, and the spatial probe is necessary to unveil nuclear and magnetization fluctuation at the nm length scale. In this contribution, I will present the advantages of magnetic small-angle neutron scattering (SANS) for investigating the nanoscale distribution of spin disorder in the relevant mesoscopic size range from 1 to a few hundred nanometres and with nanometre resolution[5]. Combining the scattering technique with complementary methods allows us to obtain a comprehensive multiscale characterization of the chemical morphology and magnetization distribution of magnetic core/shell NPs[6,7]. Specifically, by analyzing the magnetic scattering contributions, we can obtain a highly detailed internal magnetization profile of the core/shell nanoparticles. Firstly, I will present the changes in magnetization within the 2 nm ferrimagnetic shell in the FeO/Fe$_3$O$_4$, CoO/CoFe$_2$O$_4$ core/shell NPs and explore the influence of the core's magnetic state below and above the Néel temperature on the shell's magnetization response. Ultimately, I will show that magnetic SANS can disentangle the magnetization contribution from the core and shell to the total magnetization of core/shell NPs and uncover the presence of the coupling between core and shell.

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I-014

Real-space electrochemical imaging of catalytically active sites of two-dimensional materials

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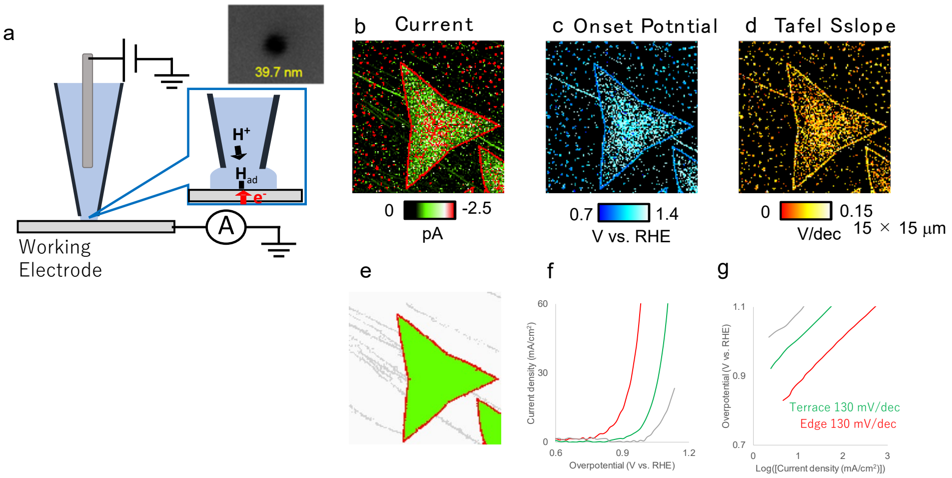
Owing to a recent increase in interest of two-dimensional (2D) layered transition-metal dichalcogenides, molybdenum disulfide (MoS_2) has received a great amount of research attention. MoS_2 is one of the most promising precious rare-metal-free catalysts for the hydrogen evolution reaction (HER). To improve the catalytic activity of MoS_2, significant efforts have been made in terms of conductivity improvement, chemical doping, phase transition, strain, and defect engineering. However, most of the research characterizes the macroscopic catalytic activity of a large number of MoS_2 nanosheets; quantitatively identifying and characterizing catalytically active sites in MoS_2 are critically important for understanding the catalysis of MoS_2. Scanning electrochemical cell microscopy (SECCM), which uses a nanopipette as a probe in a local and movable electrochemical cell, is an effective tool for characterizing surface structures electrochemically in a submicroscale spatial resolution. The advantages of SECCM are that it is a reproducible and reliable technique for fabricating nanoprobes together with fast electrochemical characterization owing to its small capacitive current and its ability to prevent sample contamination during scanning.

We have visualized inhomogeneous HER activity on a triangular 1H-MoS_2 monolayer nanosheet, heterostructures of MoS_2 and WS_2 nanosheet using SECCM(Figure 1).[1] Our data provides information about the local catalytic properties as well as electrochemical images of the HER current, Tafel slope, and overpotential by measuring the cyclic voltammograms (CVs) at all measurement points during the imaging. These SECCM measurement unveiled heterogeneous reactivity, relationship of layer number and HER activity, and aging effect. Furthermore, we succeeded in visualizing HER catalytically active sites of the Janus scroll structure MoSSe nanoscroll[2] and CO_2 reduction reaction active sites of the SnS_2 nanosheet[3]. SECCM is a powerful tool for evaluating the local catalytic activity for designing the suitable catalytic active structure and phase and can be widely applied for the characterization of 2D catalytic materials.



a) Illustration of SECCM measurements of MoS_2 nanosheets. Pd-H_2 used as a quasi-reference electrode. Nanopipette filled with 0.5 m H_2SO_4. b)–d) SECCM b) current, c) overpotential (30 mA cm^{-2}), and d) Tafel slope images of 1H MoS_2 nanosheets on HOPG substrate. Scan sizes were 15×15 μm2. Scan rate is 130 V s−1. Sweep voltage −1.3 V vs. RHE. e) MoS_2 nanosheets edge(red), terrace(green), and HOPG edge (gray) tricolor images. f),g) Graphs showing the f) overpotential and g) Tafel slope.

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Testing the precision of pseudopotentials and related methods

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Computer simulations at the level of quantum mechanics are nowadays widely used to understand a range of properties of materials or molecules and their clusters. When developing theoretical methods for simulations of materials we often focus on their accuracy. For example, more accurate density functional theory exchange-correlation functionals are being developed. However, errors due to the quality of and approximations employed in numerical set-up can be equally important. One such approximation is the use of pseudopotentials (PPs) or related methods, such as the projector-augmented-wave (PAW) scheme. Within these approaches core electrons are treated approximately which can substantially increase the speed of the calculations. For a wide range of properties this beneficial speed-up outweighs the loss of precision due to the approximate treatment of core electrons. Nevertheless, it is important to understand and quantify the loss of precision for different properties. Moreover, testing of PPs and PAWs allows one to compare different approaches that have been developed. So far, testing of PPs and PAWs focused on properties of atomic solids, such as equilibrium volumes or binding curves. However, it is difficult to extract understanding from these tests, e.g., as the number of data per element is small. Here we will show that intermolecular binding energies are very sensitive to the choice of PP or PAW dataset. This can cause substantial errors, on the order of several percent, but it can also be used to understand the errors in detail. We found that the root of the errors of binding energies due to the use of PPs or PAWs are mainly errors in the electron density. An example density error for uracil is shown in Fig. 1. We were able to devise a correction for the leading term of the error of the binding energy [1]. This correction could be used to correct calculations done with computationally cheap "soft" PPs or PAWs which would allow to reduce the computational demands or increase the system size. Moreover, we will discuss our work on extending the scheme to more elements, such as halides, and on using it for adsorption energies.

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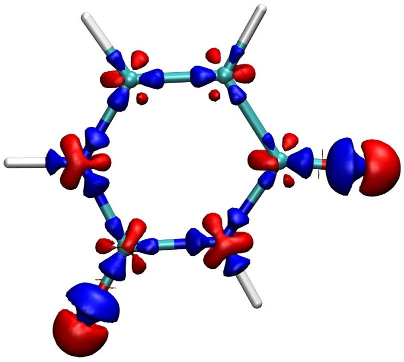

Figure 1. Electron density error for uracil molecule when so-called standard PAW datasets in VASP are used.

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I-016

Ionizing Radiation and DNA-Based Digital Data Storage

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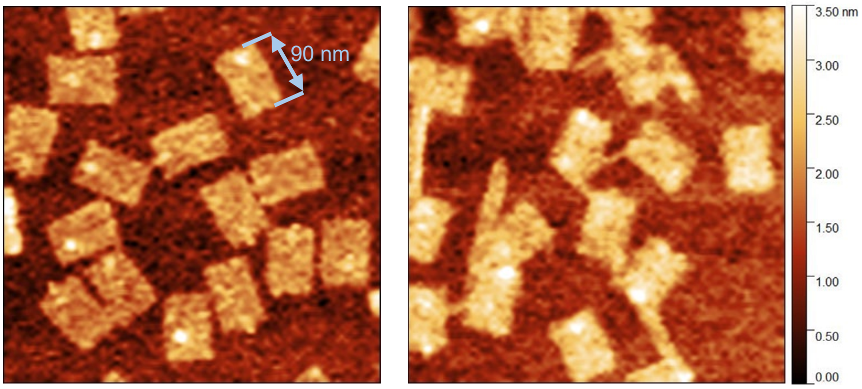
DNA-based digital data storage represents an ideal solution to data storage problems. DNA enables high data writing densities and it is stable for hundreds of years. [1] However, DNA is quite sensitive to ionizing radiation, which is known to induce DNA mutations or breaks that could be irreparable. Natural radiation sources such as radon or cosmic rays can therefore represent a significant complication in DNA-based memory development. At high data writing densities, the single ionizing radiation particle can cause damage to thousands of neighboring bits making the data unreadable by existing data reading algorithms. It is therefore important to test the radiation hardness of the structures that will be used for the digital data storage and develop protocols for safe long-term data preservation.

In our group, we are exploring details of DNA damage by ionizing radiation from very fundamental gas phase experiments [2] up to experiments with DNA sequences on DNA origami templates.[3] In a present contribution, we will report on experiments with DNA origami nanostructures that are novel candidates for the practical realization of DNA-based memory. We test their stability upon irradiation with common natural ionizing particles such as electrons, carbon, and iron ions at MeV energies. The selected DNA nanostructures show high radiation resistance, confirming their suitability for long-term data preservation applications.



Atomic force microscopy images of DNA origami nanostructures in the shape of single layer DNA rectangles with dimensions of 90x70 nm that will be used as a template for the data carrying nanostructures. Left image represents control sample of freshly synthetized DNA origami, the right image represents the sample upon irradiation with high dose (8KGy) of 16MeV electrons, where the structural distortions could be observed.

Acknowledgment: The contribution is based on the collaboration of the NEO consortium neodna.eu funded by the European Union project number 101115317. We further acknowledge the assistance provided 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.

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Moiré Multilayers — Towards Topological Quasicrystals

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Two-dimensional moiré materials exhibit a long-range moiré pattern resulting from lattice mismatch, which profoundly influences their electronic properties. In addition to the extensive study of twisted moiré bilayers in the past decade, the scope of investigation has extended to encompass multilayer systems including three or more layers. Particular attention has recently been directed toward twisted trilayer which consists of three layers arranged in a specific rotational configuration. A twisted trilayer is characterized by two distinct twist angles between adjacent layers, where the resulting multiple moiré patterns generate a quasiperiodic structure that lacks conventional periodicity.

After a brief introduction of the conventional moiré bilayer systems, we will present systematic theoretical studies on the lattice relaxation and the electronic structures in general twisted trilayer graphenes [1]. We show that the relaxed lattice structure forms a patchwork of moiré-of-moiré domains, where a moiré pattern given by layer 1 and 2 and another pattern given by layer 2 and 3 become locally commensurate (Fig. 1). The electronic band calculation reveals a wide energy window featuring sparsely distributed highly one-dimensional electron bands. These one-dimensional states exhibit a sharp localization at the boundaries between supermoiré domains, and they are identified as a topological boundary state between distinct Chern insulators. Our theoretical scheme serves as a fundamental tool and guiding principle for topological band engineering in twisted multilayers beyond graphene trilayers. Studying supermoiré multilayer systems, which offer numerous configuration possibilities, presents an opportunity to explore a new realm beyond traditional moiré bilayers.

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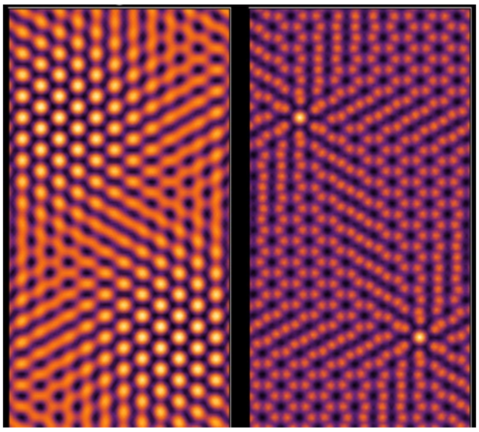

Figure 1. Moiré-of-moiré domain fomation in twisted tilayer graphene. The left and right panels illustrate the moiré pattern in the rigid and relaxed lattices, respectively.

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I-018

Optical Physics and Quantum Science using Moiré Excitonic States in van der Waals Heterobilayer

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Atomically thin low-dimensional semiconductors, such as two-dimensional (2D) transition metal dichalogenides, and nano-carbon materials have intensively studied from viewpoint of fundamental physics and potential applications [1-5,8]. The optically excitonic states with valley degree of freedom (valley exciton) and in the moiré potential (moirés exciton) provide the platform for studying novel optical physics of 2D materials. Here, I will talk about the selected topics of intriguing optical physics toward quantum science and applications arising from these novel exciton systems including moiré excitons in artificial van der Waals heterostructures [6,7,9-12].

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CHARLES UNIVERSITY
Faculty of mathematics
and physics

Charles University and the Faculty of Mathematics and Physics

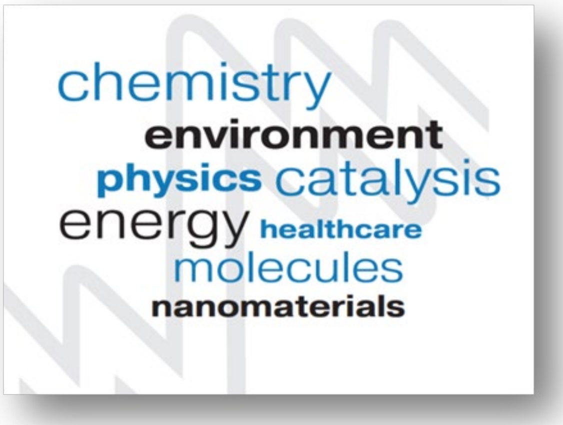
Founded in 1348 by Emperor Charles IV, Charles University (CU) in Prague is one of Europe's oldest and most prestigious universities. Over its long history, it has played a central role in the advancement of knowledge and education, becoming a global leader in various academic disciplines. Today, Charles University continues to be a prominent research institution, fostering an environment that integrates cutting-edge science, research, and education. It actively participates in knowledge transfer and commercialization through its Centre for Knowledge and Technology Transfer (CPPT), ensuring practical applications of university innovations and research through partnerships with external organizations.

The Faculty of Mathematics and Physics (MFF), established in 1952, stands at the forefront of Charles University's scientific mission. It is renowned for its rigorous academic programs and exceptional research output in a wide range of fields, including theoretical and experimental physics, fundamental and applied mathematics, and computer science. MFF's faculty members and students contribute significantly to both national and international research initiatives, positioning the faculty as a hub for scientific excellence in the Czech Republic and beyond.

MFF CU's research output accounts for approximately a quarter of Charles University's total scientific contributions. The faculty's success is underscored by its receipt of ten prestigious European Research Council (ERC) grants as of 2023, a globally recognized measure of academic and research excellence. In 2022, the faculty was involved in 46 projects within the European Union's Horizon 2020 and Horizon Europe frameworks, collectively contributing to 509 research and development projects with a budget exceeding 1 billion CZK.

MFF CU has been a crucial partner in major international projects such as the Large Hadron Collider at CERN and numerous missions with the European Space Agency. MFF CU also hosts several centers of excellence, including the Albert Einstein Center for Gravitation and Astrophysics and the Multidisciplinary Research Center for Advanced Materials (AdMat), among others. These centers, along with key national infrastructures like the Materials Growth and Measurement Laboratory (MGML), enable world-class research while fostering collaboration with industries and global research institutions.

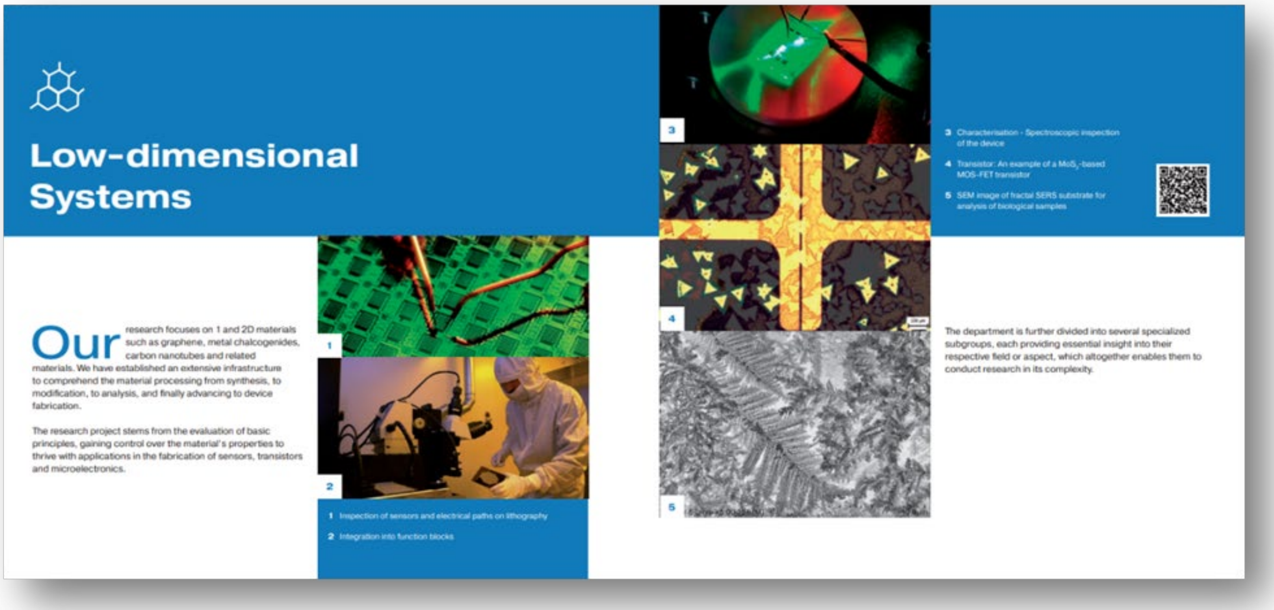
J. Heyrovský Institute of Physical Chemistry



The Heyrovský Institute of Physical Chemistry promotes the scientific legacy of the Nobel laureate, Professor Jaroslav Heyrovský, in fields related to physical chemistry. Over two hundred scientists, from promising young researchers to world-renowned experts, are engaged in groundbreaking fundamental and applied research, as well as education. Theoretically and experimentally acquired insights into physical and chemical processes are important for energy production and storage, industrial catalytic processes, healthcare and protection of the environment.

J. Heyrovský Institute of Physical Chemistry of the CAS, a public research institution, develops the scientific legacy of the Nobel Prize winner, Professor Jaroslav Heyrovský, in the fields related to physical chemistry. Over 200 scientists, ranging from promising young researchers to world-renowned top experts, are engaged in systematic basic and applied research. The theoretical knowledge and experimentally acquired knowledge of the physical chemical processes occurring in molecules and atoms are of importance for industrial catalysis, energy production and storage, health care and the environment.

The Institute operates the Heyrovský Technology Transfer Centre, which promotes cooperation between the Institute and the commercial sector in order to link the research and technological potential of the Institute with the needs of the commercial sphere.



Low-dimensional Systems

Our research focuses on 1 and 2D materials such as graphene, metal chalcogenides, carbon nanotubes and related materials. We have established an extensive infrastructure to comprehend the material processing from synthesis, to modification, to analysis, and finally advancing to device fabrication.

The research project stems from the evaluation of basic principles, gaining control over the material's properties to thrive with applications in the fabrication of sensors, transistors and microelectronics.

1 Inspection of sensors and electrical paths on lithography
2 Integration into function blocks

3 Characterisation - Spectroscopic inspection of the device
4 Transistor: An example of a MoS_2-based MOS-FET transistor
5 SEM image of fractal SERS substrate for analysis of biological samples

The department is further divided into several specialized subgroups, each providing essential insight into their respective field or aspect, which altogether enables them to conduct research in its complexity.