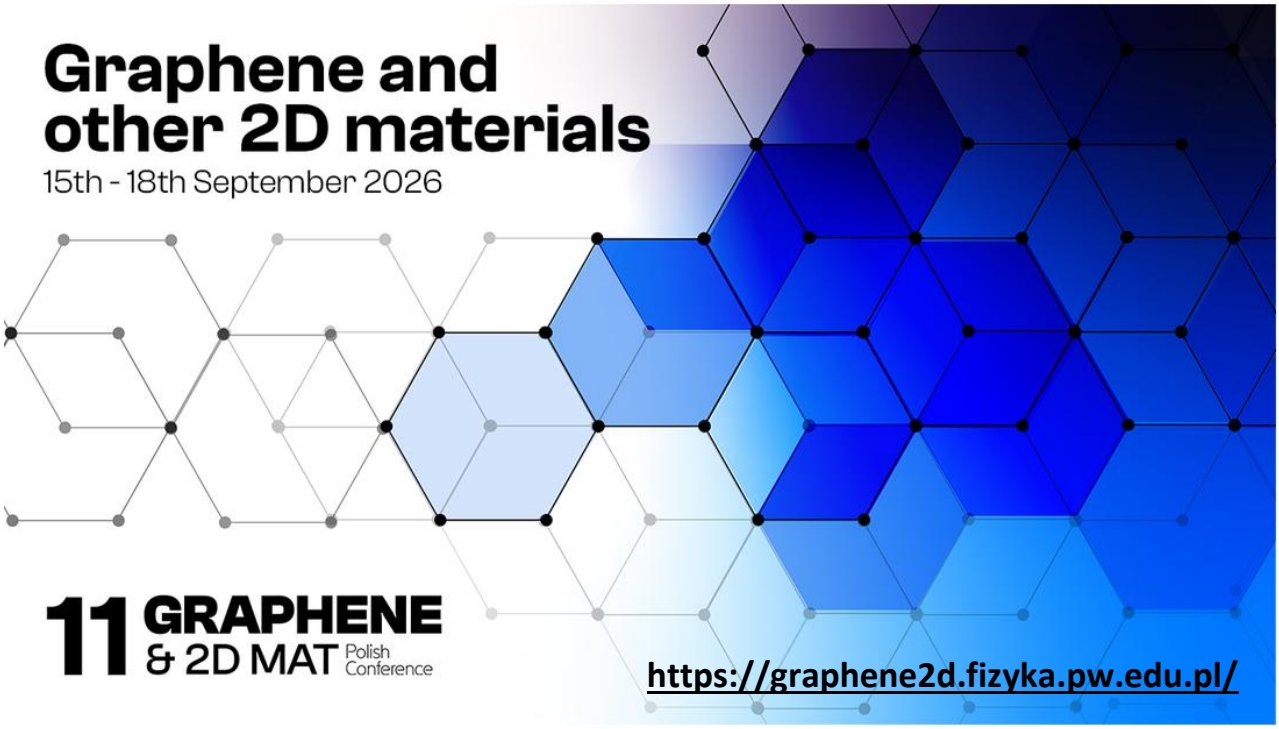


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Conference programme

Tuesday 15.09.2026

Venue: Faculty of Physics, Warsaw University of Technology (ul. Koszykowa 75)

13:00-18:00 Registration

13:50-14:00 Opening Address:

Mariusz Zdrojek, Andrzej Wysmołek

Chair: Paweł Kowalczyk

14:00-15:00 Opening Lecture

Stephan Roche: *Artificial Intelligence as main innovation driver for next generation of 2D materials and related heterostructures and composites*

15:00-15:30 Invited Talk:

Tevfik Mentes: *Deep dive into 2D materials: graphene and borophene on transition metals*

15:30-16:00 Invited Talk:

Franciszek Krok: *Self-Organized Gold Nanoislands on MoS_2: Growth, Atomic-Scale Interface Characterization and Nanomanipulation*

16:00-18:00 Welcome Reception

Wednesday 16.09.2026

Venue: Faculty of Physics, University of Warsaw (ul. Pasteura 5, room 0.06)

08:30-19:00 Registration

Chair: Mikołaj Lewandowski

09:00-09:30 Invited Talk:

Artur Ciesielski: *Beyond Graphene: 2D Materials as Next-Generation Electrode Materials for Batteries and Hybrid Supercapacitors*

09:30-10:00 Invited Talk:

Ewa Młyńczak: *Structure and Electronic Properties of Pristine 2D Materials: From Epitaxial Sn to In-Situ Exfoliated MoS_2*

10:00-10:15 Contributed Talk:

Verónica Montes-García: *Harnessing Washing-Driven Oxidation to Engineer Mo2CTx/MoOx Hybrid Interfaces for Energy Storage*

10:15-10:30 Contributed Talk:

Karolina Wenelska: *Borophene-like/NiO and influence of defects for electroactivity of oxygen evolution reaction*

10:30-11:00 Coffee break

Chair: Joanna Jadczak

11:00-11:30 Invited Talk:

Bartłomiej Graczykowski: *Brillouin Light Scattering in Low-Dimensional Systems: GHz Phonon Engineering in Quasi-2D Nanostructures and Elastic–Photoelastic Metrology of van der Waals Crystals and Membranes*

11:30-12:00 Invited Talk:

Ryszard Zdyb: *Large scale single-layer antimonene oxide*

12:00-12:15 Contributed Talk:

Mikołaj Lewandowski: *2D iron sulfide on copper: Growth, structure and properties*

12:15-12:30 Contributed Talk (Renishaw Sp. z o.o.)

Agnieszka Sozańska: *In Situ Raman–SEM Imaging for Investigating Graphene and 2D Materials in Next-Generation Li-Ion Battery Electrodes*

12:30-14:00 Lunch break

Chair session A: Maciek Molas (room 0.03a)

Chair session B: Ewa Młyńczak (room 0.06)

14:00-14:15 Contributed Talks:

Session A: Jakub Kierdaszuk: *Photoluminescence enhancement in WSe_2 doped with Nb*

Session B: Kamila Klimza: *Influence of magnetic field on the performance of 2D material-based catalysts for electrochemical water splitting*

14:15-14:30 Contributed Talks:

Session A: Ewa Żuberek: *Upconversion photoluminescence excitation reveals exciton–trion and exciton–exciton interactions in hBN/MoS_2/hBN van der Waals heterostructures*

Session B: Sonnur Kurtulus: *Low-Dimensional Borophene-Like Layer Domains Stabilized in Carbon for Electrocatalysis*

14:30-14:45 Contributed Talks:

Session A: Gayatri: *Strain induced enhanced energy transfer process in TMD heterostructures*

Session B: Karolina Pietrusewicz: *Wet ball milling in defect mediated cleavage of β-Boron for the formation of Borophene-like nanoflakes*

14:45-15:00 Contributed Talks:

Session A: Aleksandra Kasprzak: *Sign Reversal of Interlayer Exciton Valley Polarization in a WS_2/WSe_2 Moiré Heterobilayer under Sub-Gap Excitation*

Session B: Natalia Grochowska: *Tetraphenylporphyrin-grafted copolymer as a modifier for thermally conductive graphene nanoplatelet composites*

15:00-15:15 Contributed Talks:

Session A: Piotr Tatarczak: *Green Single-Photon Emitters in Epitaxial BN – Properties and Engineering*

Session B: Aleksandra Pasik: *HAp-coated nonwoven graphitic materials for regeneration of bone tissue*

15:15-15:45 Coffee break

Chair session A: Tevfik Mentes (room 0.03a)

Chair session B: Ryszard Zdyb (room 0.06)

15:45-16:00 Contributed Talks:

Session A: Zuzanna Śnioch: *Composition-Dependent Magnon Dynamics in CrSBr Mixed Crystals*

Session B: Anna Wróblewska: *Distance-Dependent Interfacial Coupling in CNT/WSe_2 mixed-dimensional Heterostructures*

16:00-16:15 Contributed Talks:

Session A: Weronika Andrzejewska: *Structural stability of 2-dimensional iron nitride islands on copper under ambient and electrocatalytic conditions*

Session B: Magdalena Kopczyńska: *Strain-Induced Optical and Electrical Properties of BN Integrated with GaN NWs*

16:15-16:30 Contributed Talks:

Session A: Julia Warowna: *Oxidation of isolated antimonene islands on W(110)*

Session B: Lena Miler: *Isotopic Effects in Epitaxial hBN: Distinguishing Hydrogen-Related Defect Complexes*

16:30-16:45 Contributed Talks:

Session A: Igor Nowik: *Nucleation engineering for homoepitaxial MOVPE growth of natBN on ^{10}BN flakes*

Session B: Tymoteusz Plak: *Towards resonant energy transfer in a $MoSe_2/ReS_2$ 2D heterostructure with tunable interlayer separation*

16:45-17:15 Coffee break

17:15-19:00 Poster Session

Thursday 17.09.2026

Venue: Faculty of Physics, University of Warsaw (ul. Pasteura 5, room 0.06)

09:00-16:30 Registration

Chair: Leszek Bryja

09:00-09:30 Invited Talk:

David Brunel: *MBE-grown PtSe2 films for thermal investigations*

09:30-10:00 Invited Talk:

Arkadiusz P. Gertych: *Measuring Thermal Properties of 2D Materials and vdW Heterostructures*

10:00-10:15 Contributed Talk:

Piotr Wojnar: *Molecular beam epitaxy of optically active indium telluride/indium selenide van der Waals heterostructures*

10:15-10:30 Contributed Talk:

Jakub Sitek: *Facile synthesis of two-dimensional amorphous carbon for enhanced corrosion resistance*

10:30-11:00 Coffee break

Chair: Marcin Syperek

11:00-11:30 Invited Talk:

Paweł Krukowski: *Single-molecule chirality: can it be identified?*

11:30-12:00 Invited Talk:

Marta Pelc: *GRANAD: A tight-binding framework for light-matter interactions and its application to mode-selective spontaneous emission*

12:00-12:15 Contributed Talk:

Karol Szałowski: *Effect of strain and electric field on charge density wave orderings in monolayer tantalum dichalcogenides: a first-principles study*

12:15-12:30 Contributed Talk:

Jacek Majewski: *Theoretical studies of plasmon and external magnetic field effects on high-harmonic generation in graphene and transition metal carbides and nitrides*

12:30-14:00 Lunch break

Chair session A: Alessandro Surrente (room 0.03a)

Chair session B: Jacek Majewski (room 0.06)

14:00-14:15 Contributed Talks:

Session A: Jan Złotopolski-Pirczewski: *Understanding piezoelectricity in epitaxial boron nitride grown by MOVPE*

Session B: Martin Lukac: *Graphene encapsulation of FeI_2 monolayer: Induced Modifications of Electronic Structure and Lattice Dynamics*

14:15-14:30 Contributed Talks:

Session A: Izabela Rogala: *Spatially correlated TEM-AFM-KPFM imaging of BN piezoelectric domains*

Session B: Subrata Rakshit: *Torsion-Driven Electronic and Magnetic Phase Transition in Boron Atomic Chains*

14:30-14:45 Contributed Talks:

Session A: Bazlul Karim: *Second Harmonic Generation Induced UV Luminescence in Rhombohedral Boron Nitride Films*

Session B: Timon Moško: *Superconducting and dielectric properties of monolayer α-$TaSi_2N_4$*

14:45-15:00 Contributed Talks:

Session A: Aleksandra Nadolska: *Local Formation of Resistive States in Ultrathin α-MoO_3*

Session B: Abhishek Ghosh: *Purcell Enhancement by the Edge States of Zig-Zag Graphene Nanoflakes*

15:00-15:15 Contributed Talks:

Session A: Bartosz Kaczmarek: *Resonant enhancement of second harmonic generation in rBN metasurfaces*

Session B: Konrad Wilczyński: *Temperature-Dependent Vibrational Properties of Monolayer WS_2 Nanocrystals: From Harmonic Phonons to Ab-Initio Molecular Dynamics*

15:15-15:45 Coffee break

Chair session A: Paweł Krukowski (room 0.03a)

Chair session B: Marta Pelc (room 0.06)

15:45-16:00 Contributed Talks:

Session A: Teresa Bizoń: *Substrate dependent properties of epitaxial BN heterostructures*

Session B: Leo Sagan: *Cross-Plane Thermal Transport in vdW Heterostructures via Joule Heating and Raman Thermometry*

16:00-16:15 Contributed Talks:

Session A: Syed Hassan Abbas Jaffery: *Pristine 2D Interfaces: Eliminating Contamination via Mechanical Sweeping*

Session B: Jakub Cwynar: *Doping of MOVPE-Grown Layered Boron Nitride: Correlation Between Doping Process and Electrical Transport Mechanisms*

16:15-16:30 Contributed Talks:

Session A: Wojciech Kolesiński: *Field induced polarization enhancement in TMD monolayer as a sensitive probe of magnetic effects in 2D heterostructures*

Session B: Gabriela Szwed: *Conductive epitaxial boron nitride: SIMS studies on acceptor activation and electrical properties*

16:15-16:30 Contributed Talks:

Session A: Bartosz Furtak: *Epitaxial boron nitride as a platform for versatile moiré heterostructures - a cathodoluminescence study*

19:00-00:00 Networking Dinner
at the Faculty of Physics, Warsaw University of Technology (ul. Koszykowa 75)

Friday 18.09.2026
Venue: Faculty of Physics, University of Warsaw (ul. Pasteura 5, room 0.06)

09:00-12:00 Registration desk

Chair: Jan Suffczyński

09:00-09:30 Invited Talk:

Bernard Gil: *Polytypism in sp^2-bonded BN*

09:30-10:00 Invited Talk:

Alessandro Surrente: *Spin injection and emission helicity switching in a BA_2PbI_4/WSe_2 heterostructure*

10:00-10:15 Contributed Talk:

Mariusz Klimczak: *Spectral shaping of SHG in hybrid hBN/rBN epitaxial stacks*

10:15-10:30 Contributed Talk:

Michał Kobecki: *Periodic Excitation of Magnons in CrSBr*

10:30-11:00 Coffee break

Chair: Piotr Kossacki

11:00-11:30 Invited Talk:

Marcin Syperek: *$MoTe_2$ for near-infrared photonics*

11:30-12:00 Invited Talk:

Maciej Molas: *Magneto-Optics of Bright and Dark Excitons in a $MoWSe_2$ Monolayer Alloy*

12:00-12:15 Contributed Talk:

Tomasz Woźniak: *Extremely High Excitonic g-Factors in 2D Crystals by Alloy-Induced Admixing of Band States*

12:00-12:15 Closing

12:30-14:00 Lunch break

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Umożliwia precyzyjne przygotowanie ultracienkich lameli do badań transmisyjnych, wykonywanie rekonstrukcji 3D heterostruktur van der Waalsa oraz mapowanie domieszek chemicznych (np. atomów azotu lub boru w sieci grafenowej) i zanieczyszczeń na powierzchni pojedynczych warstw.

SEM & TEM

Służy do szybkiej oceny ciągłości warstw, morfologii (fałd, pęcherzy) oraz – w przypadku TEM w rozdzielczości atomowej – bezpośredniego zliczania liczby warstw, identyfikacji defektów punktowych, dyslokacji oraz analizy interfejsów w nanourządzeniach.

XPS

Jest kluczowa do określania stopnia uporządkowania węgla (rozróżnienie wiązań sp^2 od sp^3), monitorowania procesu redukcji tlenku grafenu (rGO) oraz szczegółowej identyfikacji grup funkcyjnych i wiązań chemicznych po modyfikacjach powierzchniowych.

BRUKER

XRD

Precyzyjnie wyznacza odległości międzypłaszczyznowe (d-spacing), stopień krystaliczności oraz teksturę warstw, a także pozwala monitorować efekty interkalacji jonów lub cząsteczek chemicznych w przestrzenie międzywarstwowe.

XRF

Zapewnia szybką, nieniszczącą kontrolę czystości chemicznej podłoży syntezowych (np. folii metalowych do wzrostów CVD) oraz wykrywanie pozostałości katalizatorów i zanieczyszczeń metalicznych w próbkach.

AFM

Niezastąpiona przy wyznaczaniu rzeczywistej grubości płatków (monowarstwy vs. wielowarstwy) oraz jednoczesnym badaniu lokalnych właściwości nanomechanicznych, elektrostatycznych i elektrycznych (np. metodami C-AFM czy KPFM) w skali nanometrycznej.



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Book of Abstracts

(in chronological order)

Tuesday 15.9.2026

Artificial Intelligence as main innovation driver for next generation of 2D materials and related heterostructures and composites

Stephan Roche[1,2]

[1] *Catalan Institute of Nanoscience and Nanotechnology (ICN2), Bellaterra, 08193, Barcelona, Spain*

[2]*ICREA Institucio Catalana de Recerca i Estudis Avancats, 08010 Barcelona, Spain*

Up-scaling graphene and other 2D materials from the lab to products is increasingly limited by structural variability: defects, grain boundaries, interfaces, contamination, and other types of disorder that propagate from wafer fabrication to device production. The same problem exists in 2D materialsbased composites in which the multiscale nature of disorder makes optimization of their properties of true challenge.

In this talk, I will describe how physics-informed Artificial Intelligence (AI), coupled to linear-scaling (quantum) simulations, can turn this variability into a design parameter that will accelerate industrial translation. First, I will outline AI-assisted workflows that reconstruct as-grown 2D materials into atomistically faithful digital twins from multimodal characterisation, enabling direct, quantitative links between growth/process conditions and electronic, thermal and optoelectronic performance. Second, I will show how these digital twins can be used to generate surrogate models, variability-aware "design rules", and parameters for Process Design Kits (PDKs), supporting rapid co-optimization of materials, devices and circuits under manufacturing constraints. Concrete examples will include AI-guided exploration of amorphous boron-nitride compounds for nano-interconnect reliability, and digital-twin-driven assessment of polycrystalline graphene/TMDC stacks for photonics, biosensing and CMOS-compatible electronics. I will then put in perspective these capabilities in the frame of Pilot Lines which develops end-to-end prototyping services in fab environments, e.g. for integrating graphene and TMDCs into silicon platforms.

I will finish by explaining how AI-software spinoffs such as Apeiron Intelligence (www.apeironagents.tech) can provide unprecedented accelerator engine in the sense that AI-orchestrated, high-throughput digital-twin pipelines can significantly shorten iteration cycles between material design, process tuning and performance validation.

Overall, the message is significant: embedding AI-driven digital twins into pilot-line workflows and closed-loop active learning can de-risk scale-up, compress time-to-market, and strengthen the industrial competitiveness of 2D-material-enabled technologies

References

[1]Malica C, Novoselov K, Barnard AS, Kalinin SV, Spurgeon SR, Reuter K, Roche S, et al., J. Phys. Mater. 8 (2025) 021001.

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[3]Botifoll M, Pinto-Huguet I, Rotunno E, Galvani T, Coll C, Habibzadeh Kavkani P, et al., Advanced Materials (2025).

[4] Apeiron Intelligence, www.apeironai.eu

Deep dive into 2D materials: graphene and borophene on transition metals

Tevfik Onur Menteş[1]

[1]*Elettra – Sincrotrone Trieste, Basovizza, Italy*

Starting with graphene, the progress made in the field of 2D materials has given new life to surface science. In particular, the interactions between 2D layers and their support have been of great interest due to the consequences in structural, chemical, electronic and magnetic aspects of the systems under study. In this talk, we will focus on the well-studied graphene and newly-emerging borophene as the 2D layers, and give an overview of the phenomena that takes place at the interface with their underlying support. In case of graphene, the comparison between supported and suspended layers give insights on the structural [1] and electronic [2] properties of graphene. The tight graphene network and the strong bonds between carbon atoms allow for trapping foreign species at the interface with the graphene support, leading to interesting phenomena due to the extreme pressures applied by graphene to the trapped atoms and clusters [3]. Furthermore, in some cases the support goes beyond being a passive terrain, and its properties are modified due to the presence of graphene. In this respect, we will discuss the case of graphene coupled to cobalt (see Figure 1) and iron ultrathin films, for which the interface allows for engineering their magnetic properties [4,5]. Lastly, we will mention the growth of borophene networks on transition metal surfaces, and the possibility to build graphene-borophene heterostructures [6].

References

[1] A. Locatelli *et al.*, ACS Nano 4 (2010) 4879.
[2] K. Knox *et al.*, Phys. Rev. B 84 (2011) 115401.
[3] G. Zamborlini *et al.*, Nano Lett. 15 (2015) 6162.
[4] C.A. Brondin et al., Adv. Electron. Mater. 10 (2024) 2300579.
[5] C.A. Brondin et al., Carbon 249 (2026) 121169.
[6] M. Jugovac et al., Adv. Electron. Mater. 9 (2023) 2300136.

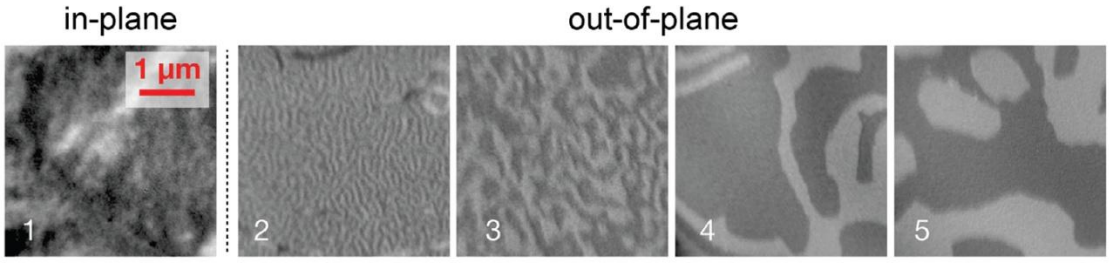


Figure 1. Magnetic domains in a graphene/Co ultrathin film grown on a Re(0001) single crystal surface. The images are acquired using x-ray magnetic circular dichorism in an x-ray photoemission electron microscope (XPEEM). The amount of graphitic carbon increases from left to right, with a subsequent strengthening of out-of-plane magnetic anisotropy in the Co film. Adapted from reference [4].

Self-Organized Gold Nanoislands on MoS2: Growth, Atomic-Scale Interface Characterization and Nanomanipulation

Franciszek Krok

Marian Smoluchowski Institute of Physics, Jagiellonian University, Łojasiewicza 11, 30-348 Kraków, Poland

The interaction between metallic nanostructures and two-dimensional materials offers a promising route toward controlled engineering of functional interfaces for molecular electronics, optoelectronics and nanoscale device architectures. In this talk, I will discuss the self-organization of gold nanoislands on MoS2 surfaces, with particular emphasis on the atomic-scale structure of the Au/MoS2 interface and its consequences for metal-substrate coupling.

Gold was deposited under ultra-high-vacuum conditions on both bulk MoS2 and synthetically grown MoS2/SiO2 substrates. Scanning tunnelling microscopy, high-resolution scanning electron microscopy and atomic force microscopy reveal the formation of epitaxial triangular Au nanoislands whose lateral size and height can be controlled by deposition temperature and coverage. The morphology and orientation of the islands reflect the crystallographic symmetry of the MoS2 substrate, indicating a well-defined epitaxial relationship between the metallic nanostructures and the layered semiconductor surface.

A central part of the presentation will focus on the atomic-scale characterization of the contact interface. Cross-sectional HAADF-STEM imaging of Au/MoS2/SiO2 structures provides direct insight into the arrangement of Au, S and Mo atomic columns at the island-substrate boundary. These measurements show that the Au structure follows the symmetry of the MoS2 lattice, while the density of Au atomic columns in the interfacial plane is lower than in the bulk of the island. This reduced interfacial density points to a weak, yet crystallographically ordered, interaction between the Au nanoislands and the MoS2 surface. In the case of supported MoS2 bilayers, the local roughness and corrugation of the underlying SiO2 substrate are transferred to the MoS2 layer, but do not prevent the epitaxial growth of Au nanoislands.

The weak and structurally well-defined Au/MoS2 contact make this system an interesting model for studying friction, commensurability and nanoscale motion on two-dimensional materials. STM and AFM experiments show that individual Au nanoislands can be displaced along preferred crystallographic directions, with their orientation preserved during manipulation. At higher coverage, collective displacement may lead to the formation of ordered stripe-like assemblies without coalescence.

Wednesday 17.9.2026

Beyond Graphene: 2D Materials as Next-Generation Electrode Materials for Batteries and Hybrid Supercapacitors

Artur Ciesielski[1,2]

[1]*University of Strasbourg & CNRS, ISIS & icFRC, 8 allée Gaspard Monge, 67000 Strasbourg, France.*

[2]*Center for Advanced Technologies, Adam Mickiewicz University, Uniwersytetu Poznańskiego 10, 61-614 Poznań, Poland.*

Two-dimensional covalent organic frameworks (2D COFs) are an emerging class of crystalline, porous materials whose well-defined molecular architecture, high surface area, and chemical tunability make them compelling electrode candidates for next-generation energy storage. Hybridizing COFs with functional materials such as metal-organic frameworks (MOFs) and polyoxometalates (POMs) further expands their accessible property space, combining the structural precision of frameworks with the redox versatility of guest species.

This talk begins with an overview of key energy storage systems, batteries and supercapacitors, and the materials-level bottlenecks that currently constrain their energy density, rate capability, and cycle life. It then surveys classical 2D materials, including MXenes [1], and transition metal dichalcogenides (TMDs) [2], as electrode materials, establishing the performance baseline and the structural limitations that motivate moving beyond them. Building on this foundation, the talk turns to the design and synthesis principles governing 2D COFs and their hybrids, including strategies for controlling crystallinity, tuning pore geometry, and installing functional groups that modulate electronic structure and electrochemical activity. I will then discuss how these structural handles translate into measurable performance gains in pseudocapacitors and in zinc- [3] and aluminum-based batteries [4], with particular attention to redox-active linkages, charge storage mechanisms, and ion transport dynamics within the porous architecture. The talk closes by situating these fundamental design principles within the broader challenge of engineering sustainable, next-generation energy storage technologies from porous framework materials.

References

[1] A. Sánchez-Oliva, V. Montes-García, Ke Li, K. Prenger, X. Guo, I.Janica, W. Kukułka, A. Tamayo, P. Prieto, P. Samorì, V. Nicolosi, A. Ciesielski, Small (2026) DOI:10.1002/smll.202507744
[2] H. Guo, V. Montes-García, H. Peng, P. Samorì, A. Ciesielski, Small 20 (2024) 2310338.
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Acknowledgments

This work was supported by the National Science Centre, Poland (Grant Number. 2024/08/X/ST5/00867, 2024/55/D/ST11/00376, 2022/47/D/ST5/00261, and 2024/55/B/ST11/00250).

Structure and Electronic Properties of Pristine 2D Materials: From Epitaxial Sn to In-Situ Exfoliated MoS_2

Ewa Młyńczak[1], Tomasz Sobol[2], Ewa Madej[1], Dorota Wilgocka-Ślęzak[1], Kinga Freindl[1], Ardra Surendran[1], Smibin Shaju[1], Olga Kowieska[1], Nika Spiridis[1]

[1] *Jerzy Haber Institute of Catalysis and Surface Chemistry Polish Academy of Sciences, Poland*

[2] *National Synchrotron Radiation Centre SOLARIS, Jagiellonian University, Krakow, Poland*

Mechanical exfoliation using Scotch tape remains one of the most widely used methods for preparing flakes of two-dimensional (2D) materials. However, its applicability to surface-science studies is limited by the small lateral size of the flakes and contamination from adhesive and polymer residues, which hinder experiments requiring large, atomically clean surfaces. Molecular beam epitaxy (MBE) together with chemical vapor deposition (CVD) provide alternative routes enabling the synthesis of selected 2D materials under controlled conditions, with MBE in particular allowing growth directly under ultrahigh vacuum (UHV) on suitable substrates. A complementary approach is the recently developed Kinetic In situ Single-layer Synthesis (KISS) technique, in which a clean single-crystal substrate is brought into contact with a freshly cleaved surface of a bulk layered material, resulting in the transfer of large-area flakes under UHV conditions [1][2].

In this talk, I will present experimental results obtained using these complementary approaches to obtaining pristine 2D materials. First, I will discuss the electronic structure of epitaxial stanene (a two-dimensional honeycomb Sn layer) grown on InSb(111). I will also present prospects for realization of stanene on alternative substrates, particularly Pt(111), discussing substrate–overlayer interactions. The Sn layers were prepared by MBE, and their electronic structure was investigated by synchrotron-based angle-resolved photoemission spectroscopy (ARPES) at the PHELIX beamline of the Solaris National Synchrotron Radiation Centre.

The second part of the talk focuses on MoS_2 flakes prepared by in situ exfoliation by the KISS technique using Pt(111). The resulting atomically clean surfaces enable high-quality ARPES measurements. Exposure of the MoS_2/Pt(111) system to ethylene leads to selective graphene formation by CVD on the bare Pt surface, while no graphene growth is observed on the MoS_2 flakes, as confirmed by ARPES. Finally, I will show that such samples are also compatible with photoemission electron microscopy (PEEM), highlighting the potential of combining spatially resolved and momentum-resolved probes for studies of pristine 2D materials.

References

[1] Y. Huang et al., Nat. Comm. 11, (2020) 2453.
[2] A. Grubisić-Čabo et al., Adv. Sci. 10 (2023) 2301243.

Acknowledgments

This work was funded by the National Science Centre, Poland (NCN), grant number 2022/46/E/ST3/00184.

Harnessing Washing-Driven Oxidation to Engineer Mo_2CT_x/MoO_x Hybrid Interfaces for Energy Storage

Verónica Montes-García[1,2], Ke Li[3], Kaitlyn Prenger[3], Xuyun Guo[3], Iwona Janica[1], Adrián Tamayo[1], Ivan Baginskiy[4], Veronika Zahorodna[4], Oleksiy Gogotsi[4], Paolo Samorì[1], Valeria Nicolosi[3] and Artur Ciesielski[1,2]

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MXenes are emerging as promising electrode materials for energy storage applications owing to their high conductivity and redox-active surfaces; [1,2] however, their propensity to undergo oxidation is often regarded as a limitation rather than an opportunity. Here, we demonstrate that the routine post-etching washing step of Mo_2CT_x, obtained via molten-salt etching, can be exploited as a controlled and tunable route to engineer Mo_2CT_x/MoO_x hybrid interfaces. By varying the duration of the post-etching $HCl/CuCl_2$ washing step (30, 90 and 240 min), we precisely tune the degree of Mo oxidation, with an additional H_2O_2 treatment serving as a reference for deliberate chemical oxidation. X-ray photoelectron spectroscopy, Raman spectroscopy and X-ray diffraction reveal two distinct oxidation mechanisms: prolonged washing induces selective Mo-centred oxidation that preserves the integrity of the carbide framework, yielding conductive Mo_2CT_x/MoO_2 domains, whereas H_2O_2 oxidation additionally affects carbon sites, producing a hydroxylated surface that compromises long-term stability. Electrochemical testing in acidic electrolyte highlights the advantages of the washing protocol: Mo_2C-90 delivers the highest specific capacitance (~150 F g^{-1} at 10 mV s^{-1}) with robust cycling stability (90% capacitance retention after 10,000 cycles), outperforming both under-oxidized (30 min), over-oxidized (240 min) and chemically oxidized (H_2O_2) counterparts. Overall, this work establishes washing-induced oxidation as a simple, scalable strategy to tailor the surface chemistry of Mo_2CT_x MXenes, transforming a standard purification step into a deliberate tool for performance optimization in supercapacitor applications.

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This work was supported by the European Union and the National Science Centre, Poland (grant no. 2023/51/B/ST11/00504).

Borophene-like/NiO and influence of defects for electroactivity of oxygen evolution reaction

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Two-dimensional (2D) materials have emerged as a rapidly expanding class of nanomaterials owing to their exceptional physicochemical properties and broad application potential in energy conversion, storage, sensing, and catalysis. Following the remarkable success of graphene, borophene has attracted increasing attention due to its high electrical conductivity, tunable electronic structure, and outstanding catalytic properties. These characteristics make borophene a promising candidate for next-generation electrochemical devices.

This work presents a comprehensive study of borophene-like development from β-boron as a bulk precursor via liquid assisted ultrasound process, its functionalization with NiO and defect formation to its application as an efficient electrocatalyst for the oxygen evolution reaction (OER).

Ex situ characterization using XPS, XRD, EPR, and nitrogen adsorption analyses demonstrated that these structural features promote both the conventional adsorbate evolution mechanism and the lattice oxygen-mediated mechanism during OER. Electrochemical measurements revealed outstanding catalytic activity, with an overpotential of only 169.56 mV at 10 mA cm^{-2} and a Tafel slope of 31 mV dec^{-1} in 1 M KOH, outperforming commercial RuO_2 and the majority of recently reported OER electrocatalysts.

The presented results demonstrate that the combination of scalable borophene synthesis and rational defect engineering offers an effective strategy for developing advanced electrocatalysts for sustainable energy conversion technologies, highlighting β-boron derived flakes as a highly promising material for future renewable energy applications.

Acknowledgments

This research has received funding from the National Science Centre (Poland) with grant OPUS21 number (2021/41/B/ST5/03279).

Brillouin Light Scattering in Low-Dimensional Systems: GHz Phonon Engineering in Quasi-2D Nanostructures and Elastic–Photoelastic Metrology of van der Waals Crystals and Membranes

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Low-dimensional materials allow GHz phonons/hypersounds to be controlled through confinement, interfaces, strain, and periodicity. However, this requires reliable elastic and photoelastic data, which remain scarce for van der Waals (vdW) systems, particularly between bulk crystals and few-layer membranes.

In this talk, I will show how spontaneous micro-Brillouin light scattering (BLS) provides a contactless route to both mechanical metrology and phonon engineering. The measured frequency shifts give phonon velocities and dispersion at selected wavevectors, while polarization-resolved intensities probe refractive and photoelastic anisotropy.

I will first discuss α-MoO_3, a transparent and strongly anisotropic vdW crystal. Angle- and polarization-resolved BLS enables determination of its acoustic and elastic anisotropy and provides access to the direction-dependent photoelastic response. I will then present freestanding 2H-$MoSe_2$ membranes, where micro-BLS reveals systematic elastic softening toward the few-layer limit and simultaneously provides information on elasticity, residual stress, and thickness [1].

Finally, I will extend this approach to quasi-2D phononic systems. In thin membranes, confinement produces guided acoustic modes, whereas periodic perforation, mass loading, or colloidal assembly can reshape their dispersion through band folding, local resonances, and mode hybridization [2,3]. These examples show how BLS connects quantitative material characterization with GHz phonon engineering, from vdW crystals and few-layer membranes to two-dimensional phononic crystals.

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Acknowledgments

This work was supported by the National Science Centre, Poland (NCN), under the SONATA BIS grant UMO-2024/54/E/ST3/00232.

Large scale single-layer antimonene oxide

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The development of future electronics based on sub-3-nm technology imposes extremely stringent requirements on the dielectric layers used in electronic components [1]. Insulating layers with thicknesses below 1 nm must meet several key criteria, the most important of which are a wide bandgap and a high dielectric constant. Equally important is the structural quality of the dielectric layer, which should be continuous and highly crystalline. Among the candidate materials, antimony trioxide, with a bandgap of 3.5 eV and a dielectric constant of $k = 6$, fulfills the key requirements for this class of dielectric materials.

Here, we report the formation of a single-layer antimony trioxide film on a tungsten surface. The oxide is synthesized by exposing a monolayer of α-phase antimonene [2] to ambient conditions. A highly ordered crystalline oxide is subsequently obtained by gentle annealing of the film under ultrahigh vacuum (UHV) conditions. The very good crystallographic order is confirmed by low-energy electron diffraction (LEED), which reveals sharp diffraction spots. The lattice constant of the layer corresponds to the Sb_2O_3 phase. LEED measurements further show that the oxide film consists of six in-plane rotational domains. Angle-resolved photoemission spectroscopy (ARPES) reveals flat electronic bands below the Fermi level, confirming the formation of an insulating layer on the metallic tungsten substrate [3]. LEED, ARPES, and low-energy electron microscopy (LEEM) demonstrate the formation of a large-area oxide film of the order of cm^2.

Interestingly, the oxide layer transforms back into α-phase antimonene upon further annealing under UHV conditions. This transformation is evidenced by the disappearance of the diffraction spots associated with antimony trioxide and the simultaneous emergence of the characteristic antimonene diffraction pattern. It is further confirmed by X-ray photoelectron spectroscopy (XPS), which initially shows spectral features characteristic of antimony oxide that progressively disappear during annealing.

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The work has been supported by the National Science Centre (Poland) under Grant No. 2024/55/B/ST11/01717.

2D iron sulfide on copper: Growth, structure and properties

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Metallic iron and iron compounds, such as iron oxides, carbides, sulfides and nitrides, are well-known for their unique electronic, catalytic and magnetic properties. These properties may be further fine-tuned by growing the material epitaxially in a 2-dimensional form on a single-crystal substrate. We have succesfully grown 2D islands of iron sulfide on Cu(001) using the approach developed by another group for MoS_2 on Cu(111) [1]. The procedure includes exposing the copper substrate to thiophenol (C_6H_6S) vapor, depositing Fe and annealing in ultra-high vacuum (UHV). The obtained islands are reconstruction-free and represent the metallic and non-magnetic FeS phase, as confirmed by scanning tunneling microscopy (STM), low energy electron diffraction (LEED), X-ray photoelectron spectroscopy (XPS) and density functional theory (DFT) [2].

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In Situ Raman–SEM Imaging for Investigating Graphene and 2D Materials in Next-Generation Li-Ion Battery Electrodes

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Graphene and other two-dimensional (2D) materials are promising functional components for advanced lithium-ion battery electrodes, offering high electrical conductivity, large surface area and mechanical flexibility. Their performance, however, strongly depends on their spatial distribution, structural properties and interactions with the electrochemically active material.

In this work, we present ***in situ*** **Raman–SEM** solution for the characterization of carbon/graphene-based electrode architectures. Raman spectroscopy provides direct structural information on graphene through its characteristic D, G and 2D bands, while SEM enables simultaneous visualization of the electrode microstructure. Raman mapping further allows the spatial distribution of graphene and 2D materials to be correlated with individual electrode particles and morphological features.

The approach provides a powerful multimodal methodology for investigating graphene-containing electrodes, including graphene/NMC and graphene/silicon architectures, and for monitoring structural changes during electrochemical operation. The combination of chemical and structural information from Raman spectroscopy with high-resolution SEM imaging offers new possibilities for understanding the role of graphene and other 2D materials in improving charge transport, structural stability and cycling performance.

The presented methodology highlights the potential of **inLux-Raman-SEM** as a powerful analytical platform for the development and optimization of next-generation graphene-enabled energy-storage materials.

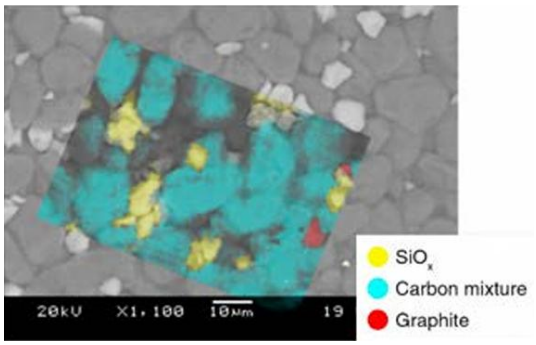


Figure 1. Correlative SEM and Raman images of a carbon-coated battery anode illustrating the distribution of different forms of carbon and silicon.

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Wednesday 17.9.2026

Afternoon Session A

Photoluminescence enhancement in WSe_2 doped with Nb

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Transition metal dichalcogenides (TMDs) offer a broad range of applications in optoelectronics, sensors, energy devices, and photovoltaics.[1] Their main weakness is doping. The two-dimensional structure of TMDs results in a high ionisation energy of impurities, so a high dopant concentration, around a few per cent, is required to affect their carrier concentration.[2] Some authors claim that such a high dopant concentration may quench the photoluminescence (PL) of TMDs due to an increased density of positive trions.[3] In our work, we found that the PL of WSe_2 is strongly enhanced by Nb doping. The PL enhancement ratio by two orders of magnitude is present over the temperature range from 5 K to room temperature. This effect is strong not only in the monolayer (Fig. 1(a)) but also in the bilayer (Fig. 1(b)) and trilayer. Unexpectedly, the PL intensity of the doped 2L of WSe_2 is stronger than that of the undoped 1L. Furthermore, the Nb doping results in the strongest enhancement of the band at 1.6 eV. This observation suggests that the Nb dopant may change the spin state of the WSe_2 valence bands, thereby making the dark ground state of WSe_2 bright. One piece of evidence is an exceptionally strong dark exciton line in 1L WSe_2 doped with Nb and encapsulated in hBN. Therefore, our results show that, contrary to some reports, doping of TMDs without decreasing their PL intensity is possible.

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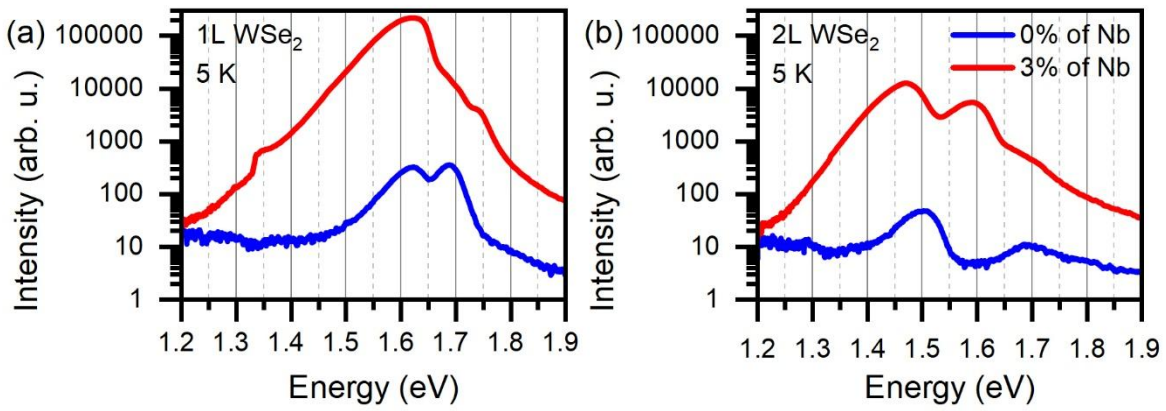


Figure 1. Photoluminescence spectra of pure WSe_2 (blue) and doped with 3% of Nb (red), measured at 5 K for:

(a) 1L WSe2, and (b) 2L of WSe2.Spectra are present on a logarithmic scale.

Upconversion photoluminescence excitation reveals exciton–trion and exciton–exciton interactions in hBN/MoS_2/hBN van der Waals heterostructures

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Transition-metal dichalcogenide monolayers, characterized by a direct band gap at the K^-/K^+ points of the Brillouin zone, are promising candidates for optoelectronic and spintronic applications due to their strong Coulomb interactions and distinctive spin-valley properties. In addition, they provide an excellent platform for investigating both electronic and phononic interactions as well as intra- and intervalley excitonic complexes [1, 2].

Here, we investigate excitonic complexes by photoluminescence upconversion spectroscopy (UPC PLE) in hBN-encapsulated MoS_2 monolayers with relatively low electron doping. The regular and upconverted PL recorded at 7 K is shown in Fig. 1. UPC PLE spectra were obtained by monitoring the neutral exciton PL while tuning the excitation energy across the low-energy side of the trion resonance (−25 to −45 meV relative to X_A). The integrated UPC PL and corresponding color maps reveal a maximum energy gain of ~45 meV that remains unchanged up to 100 K. As this value is comparable to the E_2g optical phonon energy in MoS_2, we attribute the observed upconversion to a single-phonon process. Under resonant excitation of $X_{A(1s)}$, we additionally observe emission from the excited states $X_{B(1s)}$ and $X_{A(2s)}$, located up to 160 meV and 190 meV above the excitation energy, respectively. These large energy gains suggest the involvement of many-body interactions, including exciton–exciton (Auger) scattering processes characteristic of TMD monolayers involving an excited conduction band [3].

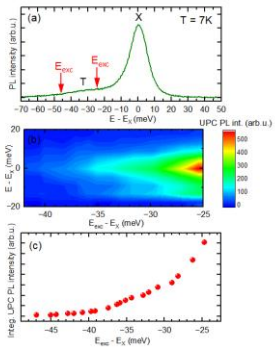


Figure 1. (a) PL spectrum of the hBN/MoS_2/hBN heterostructure measured at 7 K. (b) Color map of the UPC PLE spectra. (c) Integrated UPC PL of the neutral exciton.

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Strain induced enhanced energy transfer process in TMD heterostructures

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Two-dimensional (2D) transition metal dichalcogenides (TMDs) stacked into type-II heterostructures (HSs) exhibit competing interlayer relaxation pathways. Using an hBN spacer suppresses charge transfer and promotes Förster-type energy transfer (ET) [1]. Such ET is governed by interlayer distance, spectral overlap and excitonic dynamics, but its tunability via strain remains unexplored. In this work, we investigate strain-controlled ET in a 1L ReS_2-hBN-1L $MoSe_2$ HS transferred onto hBN bubbles [Fig. 1 (a)]. The bubbles, generated in MOVPE-grown hBN, introduce biaxial tensile strain in the layers. This reduces the bandgaps of both ReS_2 and $MoSe_2$, and a large number of carriers in both layers increases the dipole-dipole interactions. This enhances the ET from ReS_2 to $MoSe_2$ in the strained HS. As a result, the unstrained HS shows only ~2-fold enhancement in $MoSe_2$ emission compared to the unstrained 1L $MoSe_2$, whereas the strained HS shows ~5-fold enhancement as shown in Fig. 1 (b) & (c) by PL mapping, through bandgap renormalization and enhanced carrier injection. This leads to more efficient ET and amplified radiative recombination in $MoSe_2$. Overall, such strain-controlled ET offers new opportunities for tunable optoelectronic devices.

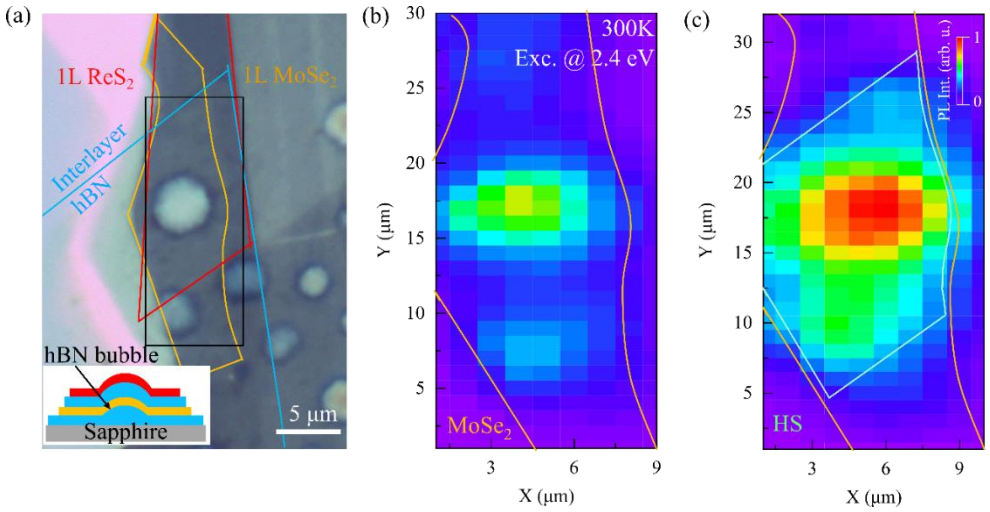


Figure 1. a) Optical image of the sample with cross-sectional schematics. The black box indicates the region selected for PL mapping. b) PL map measured at 300 K with excitation energy 2.4 eV, showing enhanced $MoSe_2$ emission due to the strain induced by bubble, c) $MoSe_2$ emission further enhanced significantly in the HS region due to the enhanced interlayer ET.

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Sign reversal of interlayer exciton valley polarization in a WS_2/WSe_2 moiré heterobilayer under sub-gap excitation

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Properties of heterostructures made of monolayers of transition metal dichalcogenides make them a rich platform for exploring correlated many-body phenomena in semiconductor physics [1]. Moiré superlattices in TMD heterobilayers host interlayer excitons whose valley degree of freedom is governed by the quasi-angular momentum of the trapping site [2], yet conventional above-gap excitation accesses these 50–230 meV below the WSe_2 A-exciton resonance, to create interlayer excitons directly in an R-type WS_2/WSe_2 moiré heterobilayer at 7 K. Power-driven sign reversal of the degree of circular polarization of the IX_1 ground state is observed, from −9% to +12%, absent under above-gap conditions. A spectral threshold at 1.577 eV separates two regimes with opposite valley injection: magneto-photoluminescence confirms the same emitting state in both regimes, but reversed valley population imbalances, which provide direct evidence for coexisting moiré miniband states with co-circular and crosscircular selection rules. A rate-equation model quantitatively reproduces the sign reversal through nearly symmetric injection, exchange depolarization, chiral-phonon intervalley scattering, and biexciton-mediated valley purification. Sub-gap excitation spectroscopy thus opens a direct spectroscopic window into the excitonic miniband structure and valley-contrasting selection rules of moiré superlattices.

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Green Single-Photon Emitters in Epitaxial BN – Properties and Engineering

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Two-dimensional boron nitride (BN) hosts room-temperature single-photon emitters (SPEs), making it a promising material for quantum photonic devices. Most studies focus on exfoliated BN flakes, which are unsuitable for applications due to limited scalability and reproducibility. This issue might be addressed by metal-organic vapor phase epitaxy (MOVPE), which enables wafer-scale BN growth [1,2] and supports the incorporation of carbon-related quantum emitters by the use of organic precursors such as triethylboron (TEB) [3,4]. However, up to now, studies on SPE formation during epitaxy remain limited.

To address this issue, in this work, we statistically analyze the influence of MOVPE growth conditions on the properties of BN-based SPEs emitting in the green spectral range. When the TEB flow rate exceeds a threshold value, we observe a crossover from a growth regime that favors the generation of SPEs to one in which formation of defect ensembles becomes dominant. In addition, a BN layer must be sufficiently thick to ensure the stability of most emitters. Our results provide quantitative limits on the organic precursor flow rate and BN thickness required to generate high-quality SPEs for future quantum devices.

Both these parameters also affect emitter density, making its optimization challenging. To simplify this task, based on experimental observations, we introduce a simple model describing emitter concentration as a function of a single effective parameter that incorporates both the BN thickness and the TEB flow rate (Fig. 1). Since only one parameter needs to be adjusted, the proposed approach significantly simplifies emitter-density optimization and may facilitate the development of scalable BN-based quantum devices.

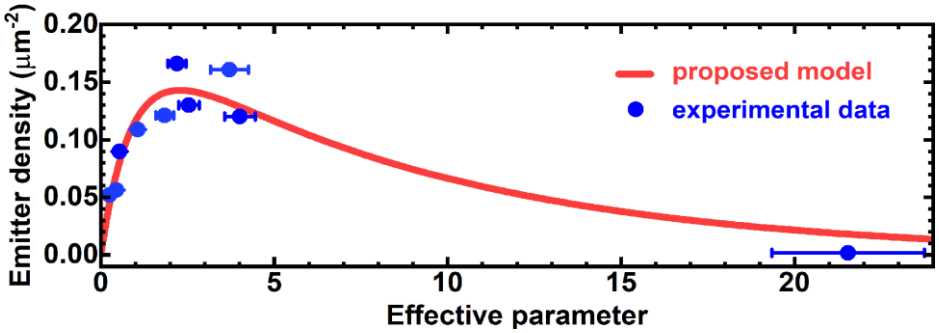


Figure 1. Spatial density of the observed green emitters in a function of the introduced effective parameter.

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Acknowledgments

This work has been partially supported by the National Science Centre Poland under decisions 2020/39/D/ST7/02811 and 2022/45/N/ST7/03355

Composition-Dependent Magnon Dynamics in CrSBr Mixed Crystals

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The discovery of intrinsic two-dimensional magnets and their integration into van der Waals heterostructures have expanded the landscape of collective phenomena in reduced dimensionality systems. Of particular interest are coherent magnons – elementary spin-wave excitations of an ordered magnetic lattice – which provide a platform for optically probing spin dynamics. This approach is especially compelling in materials that combine long-range magnetic order with semiconducting character, such as CrSBr, whose intrinsic band gap enables direct optical access to spin-related excitations[1].

To explore the tunability of magnetic and optical properties beyond those of the pristine CrSBr we employ mixed-crystal engineering approach, which provides a direct means of modifying magnetic interactions within a single crystalline phase. In CrSBr, partial substitution of Br with Cl enables controlled modification of exchange parameters and magnetic anisotropy while preserving the layered structure. Here, we investigate whether gradual chemical substitution preserves the long-range magnetic order of the parent compound, e.g., in terms of the magnon spectrum and its magnetic-field evolution.

In this work we study magnon excitations using two-color femtosecond pump–probe spectroscopy, which provides high-resolution access to coherent spin dynamics at low temperatures and high magnetic fields. In particular, we investigate how magnon frequencies evolve with chemical composition and external magnetic field in mixed CrSBr crystals. By systematically varying the halogen content, we track composition-dependent shifts of spin-wave modes and their field response, revealing changes in exchange interactions and magnetic anisotropy induced by controlled substitution. We find that the resulting tunability of the magnon frequency exceeds a factor of 2x, and the change follows virtual crystal approximation.

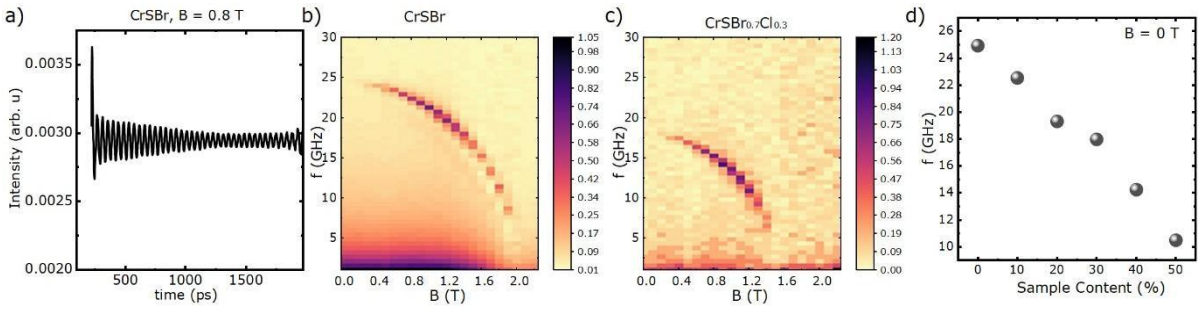


Figure 1. a) Oscillatory part of transient optical reflectivity as a function of pump–probe delay. **b-c)** Magnon dispersion map of CrSBr and $CrSBr_{0.7}Cl_{0.3}$ obtained by Fourier transform of the data in a for a different magnetic fields, **d)** Zero field frequencies as a function of sample content.

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Structural stability of 2-dimensional iron nitride islands on copper under ambient and electrocatalytic conditions

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Iron nitrides constitute an interesting group of synthetic materials with a very rich phase diagram [1]. In the bulk form, they exhibit superior mechanical, electronic and magnetic properties, which make them applicable in various industrial fields. Recently, attention has been paid to low-dimensional forms of these compounds, which are interesting from the point of view of heterogenous catalysis. We have epitaxially grown 2-dimensional iron nitride islands on a single-crystal copper substrate and studied the structural stability of the system under ambient and electrocatalytic conditions. The islands constitute a 2D representation of the γ'-Fe_4N iron nitride phase, resembling the middle-plane-cut of the bulk unit cell, with additional surface N atoms [2]. Exposing the system to ambient conditions leads to the transformation of iron nitride to iron oxynitride, however, the overal morphology remains intact. Further exposure to electrocatalytic conditions (acidic, basic or neutral – with an oxidizing or reducing potential) leads to the decomposition of iron nitride and oxidation of the underlying copper substrate. The obtained results provide valuable insights into the potential application of iron nitrides in electrocatalytic hydrogen evolution and oxygen evolution reactions (HER/OER).

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The studies were financially supported by the Foundation for Polish Science through the First TEAM/2016-2/14 project No. POIR.04.04.00-00-28CE/16-00 and the Proof of Concept (PoC FENG) project No. FENG.02.07-IP.05-0214/23 co-funded by the European Union under the European Regional Development Fund and within the European Funds for Smart Economy (FENG) programme, respectively. The authors also thank the National Science Centre of Poland for financing through the SONATA BIS project No. 2023/50/E/ST3/00704. W.A. additionally acknowledges AMU for the financial support through the "The Excellence Initiative – Research University" (ID-UB) programme within the project No. 140/04/POB3/0025 (call No. 140 "50×50: fifty grants for fifty young scientists").

Oxidation of isolated antimonene islands on W(110)

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The intensive research on two-dimensional (2D) pnictogen group materials (P, As, Sb, Bi) is driven by the need of modern, semiconducting materials for new-generation electronic systems. Among these, antimonene, a 2D allotrope of antimony, appears highly stable under ambient conditions. However, there is still an ongoing debate regarding its reactivity to air compounds. Depending on the source, antimonene exhibit: i) inertness [1]; ii) oxidation of topmost layers [2]; iii) complete oxidation [3] on the air. The LEEM (Low-Energy Electron Microscopy) and LEED (Low-Energy Electron Diffraction) results presented in this talk demonstrate dependency of antimonene oxidation on its thickness and allotropic form.

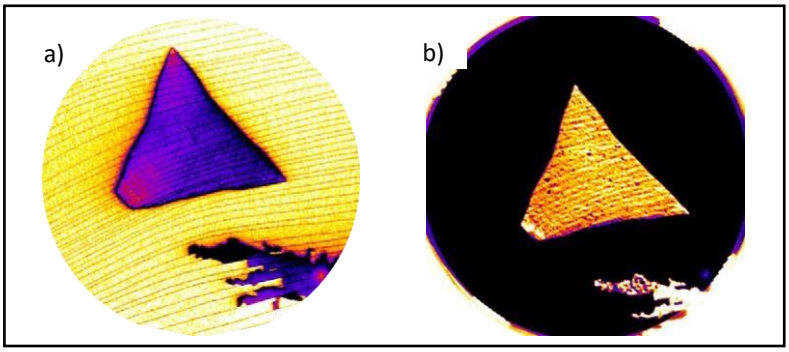


Figure 1. LEEM images of multilayer β-Sb isolated island a) before oxidation FoV = 4 µm, E = 2.8 eV and b) after oxidation and annealing FoV = 4 µm, E = 2.8 eV. The change of contrast is caused by oxidation and annealing process.

The study continues the detailed analysis of oxidation process of antimonene layers epitaxially grown on a W(110) substrate [4]. The three-stage experiment included analysis of isolated Sb islands: i) before oxidation; ii) right after air exposure; iii) after post-exposure annealing. Evolution of antimonene islands after each stage was observed by LEEM and LEED. LEEM allowed for the real-time observation of sample surface morphology while LEED enabled observation of structural transitions of antimonene. The presented results constitute a structural description of the influence of oxidation process on multilayer antimonene isolated islands.

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The work has been supported by the National Science Centre (Poland) under Grant No. 2024/55/B/ST11/01717.

Nucleation engineering for homoepitaxial MOVPE growth of ^{nat}BN on ^{10}BN flakes

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Boron nitride (BN) is a 2D material that can be obtained using various crystal growth techniques, such as Metal-Organic Vapor Phase Epitaxy (MOVPE) [1]. Epitaxial growth on sapphire substrates is promising, though it creates material of lower quality than the bulk crystals. A reasonable solution is homoepitaxy on BN flakes exfoliated from bulk crystal onto sapphire. Still, nucleation on atomically smooth surfaces of such flakes poses a challenge [2,3]. It has been shown that MOVPE growth on BN flakes causes homoepitaxial material to accumulate preferentially at the edges of exfoliated flakes [4], as well as around cracks and structural defects. However, we aim to grow uniform BN layer on the entire, atomically smooth surface of the flake and thus it is essential to develop a strategy for efficient nucleation. This can be achieved by various pre-growth procedures that include plasma treatment and etching in mixed ammonia and hydrogen atmosphere within the MOVPE reactor. When performed correctly, these steps allow for creation of triangular etch pits on previously atomically smooth BN flakes that subsequently serve as nucleation centers for MOVPE BN growth. In our study, ^{nat}BN is grown on isotopically purified ^{10}BN flakes exfoliated from bulk crystal [4]. This allows us to differentiate epitaxially grown material from the bulk flake with the use of Raman spectroscopy, due to differences in boron masses leading to distinct positions of characteristic bands for boron nitride with natural boron and ^{10}B.

In this communication, we show how different parameters of pre-growth treatment affect ^{10}BN flakes which in turn influences homoepitaxy of ^{nat}BN. Emphasis will be placed on the results obtained from Raman spectroscopy and Atomic Force Microscopy (AFM). This analysis allows us to determine optimal strategy for efficient nucleation and to evaluate crystal quality of homoepitaxially grown material.

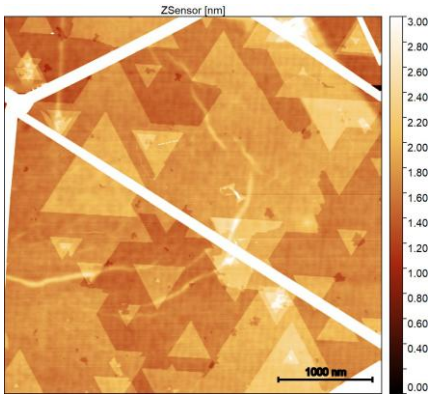


Figure 1. An Atomic Force Microscopy topography picture of MOVPE-grown ^{nat}BN on ^{10}BN flake. Homoepitaxially grown ^{nat}BN triangles can be seen on the entire surface of the flake.

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This work was supported by the National Science Centre, Poland under decision 2024/55/D/ST5/02892.

Wednesday 17.9.2026

Afternoon Session B

Influence of magnetic field on the performance of 2D material-based catalysts for electrochemical water splitting

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Magnetic field-assisted electrocatalysis has attracted significant interest as a novel approach to enhancing green hydrogen production[1,2]. While various two-dimensional (2D) materials have already been investigated as catalysts for the hydrogen and oxygen evolution reactions (HER, OER), integrating them with an external magnetic field offers a new framework for evaluating and boosting their performance[3,4].

In this work, the influence of a constant magnetic field on reaction kinetics and mechanisms was investigated using a standard three-electrode system. The working electrodes were fabricated from a magnetic composite based on 2D materials. Electrochemical performance was evaluated via cyclic voltammetry (CV), linear sweep voltammetry (LSV), and electrochemical impedance spectroscopy (EIS). Furthermore, these electrochemical insights were correlated with structural and surface alterations characterized using EPR, XPS, XRD, SEM and TEM.

This research offers insights into how electrochemical water splitting can be tuned via external factors. Consequently, it can advance the development of more sustainable energy technologies.

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This work was supported by Rector of the West Pomeranian University of Technology in Szczecin for PhD students of the Doctoral School, grant number: ZUT/17/2026.

Low-Dimensional Borophene-Like Layer Domains Stabilized in Carbon for Electrocatalysis

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Borophene has emerged as a promising two-dimensional material owing to its metallic character, anisotropic electronic properties, and potential for energy conversion. However, its practical application remains limited by oxidation, structural instability, and restacking under ambient conditions [1].

Here, we report a scalable strategy for stabilizing borophene-like layers within a porous carbon matrix through surfactant-assisted polymerization followed by carbonization, as schematically illustrated in Figure 1. TEM, SEM-EDS, Raman spectroscopy, and nitrogen adsorption analysis confirm the preservation of lamellar borophene-like layers embedded in a conductive hierarchical porous carbon framework. The composite exhibits a specific surface area of 728 $m^2\ g^{-1}$, significantly higher than that of the borophene-free reference material [2].

The resulting material demonstrates bifunctional electrocatalytic activity, delivering an ORR onset potential of 0.85 V versus RHE in alkaline electrolyte and an HER overpotential of 374 mV at 10 mA cm^{-2} with a Tafel slope of 125 mV dec^{-1} in acidic electrolyte.

These findings suggest that confining borophene-like layer domains within a conductive carbon matrix modifies the local electronic structure of B–C active sites and enhances charge transfer during electrochemical reactions. This work combines experimental observations with first-principles DFT calculations to elucidate the electronic structure of borophene–carbon interfaces and the adsorption of ORR and HER intermediates.

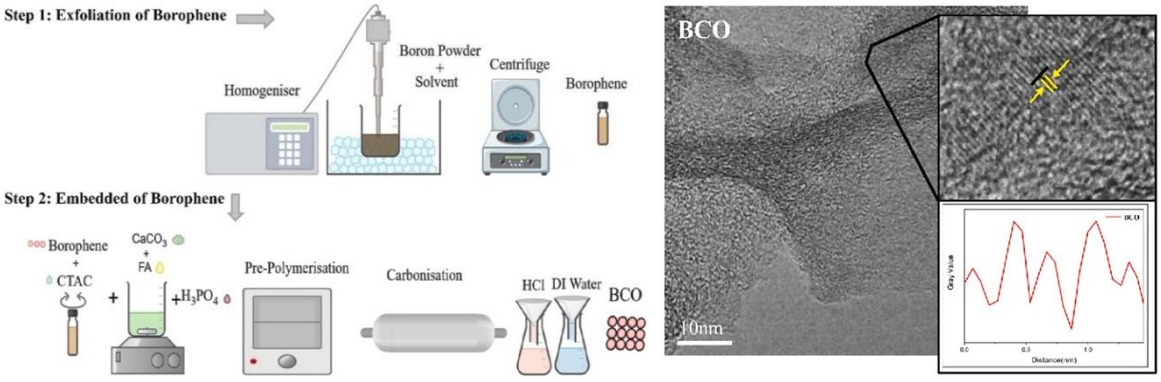


Figure 1. Schematic illustration of the fabrication process for stabilized borophene-like layer domains embedded in a carbon matrix, together with a representative TEM image of the resulting composite.

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Wet ball milling in defect mediated cleavage of β-Boron for the formation of Borophene-like nanoflakes

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Two-dimensional boron-based materials, commonly referred to as borophene, have attracted considerable attention due to their anisotropic structure, metallic character and potential applicability in catalysis, energy conversion and nanoelectronics [1]. In comparison with other two-dimensional materials, borophene exhibits a unique combination of high electrical conductivity, mechanical flexibility and rich variety of structures, making it promising candidate for next generation functional materials. Despite these attractive, the scalable preparation of borophene and borophene-like nanostructures remains challenging.

Among the alternative approaches, liquid-phase methods have emerged as attractive routes due to their simplicity, scalability and relatively low cost. In such processes, the choice of solvent plays a crucial role, as it directly affects the particle–solvent interactions, exfoliation efficiency and colloidal stability. Since solvent selection is one of the key factor governing the efficiency and stability of exfoliaton in liquid phase of 2D materials, understanding the influence of solvent properties is crucial for optimizing the production of boron-based nanosheets [2].

In this work, wet ball milling was investigated as a path for the preparation of few-layer borophene-like nanosheets from β-boron powder. The process was carried out in different solvent environments, including isopropanol, ethanol, n-hexane and acetonitrile. The prepared materials were examined using methods like X-ray Diffraction (XRD), Atomic Force Miscorcopy (AFM) and Transmission Electron Miscroscopy (TEM).

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Tetraphenylporphyrin-grafted copolymer as a modifier for thermally conductive graphene nanoplatelet composites

Natalia Grochowska,[1,2] Konrad Wilczyński,[2] Agnieszka Kuklewska,[1] Dariusz Baran,[1] Maciej Malinowski,[1] Urszula Ulkowska,[1] Piotr Wieciński,[1] Anna Czajka-Warowna,[3,4] and Andrzej Plichta[1]

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The Graphene Flagship Technology and Innovation Roadmap identifies graphene-filled polymer composites as the area of graphene application closest to real-world implementation [1]. Despite this promise, the design and manufacturing of such materials still pose significant challenges. In thermally conductive composites, intended for heat management in electronic devices, these challenges include not only the high viscosity of compositions and the risk of filler agglomeration or uncontrolled spatial orientation but also heat carrier scattering at the filler-matrix interfaces. Literature reports multiple strategies to mitigate the resulting interfacial thermal resistance by altering interactions between the phases. However, most of them require covalent bonding with the filler, which creates new scattering sites and decreases filler's intrinsic thermal conductivity [2].

In this study, we propose a macromolecular additive that acts as a bridge between the graphene-related filler and the polymeric matrix. Non-covalent interactions between the carbon layers and the additive's side groups ensures that the crystalline structure of the filler stays intact. At the same time, the use of polymers of opposing chirality allows the additive and the matrix to cocrystallize. The strategy limits the number of factors influencing composite properties and facilitates the interpretation of the observed phenomena.

We discuss challenges in the use of commercial graphene nanoplatelets in the context of their interactions with tetraphenylporphyrin derivatives, supporting the interpretation of experiments with DFT simulations. In the synthetic part, we identify limitations arising from the structure of tetraphenylporphyrin and show how they can be overcome. Finally, we demonstrate how the obtained additive affects composite performance.

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HAp-coated nonwoven graphitic materials for regeneration of bone tissue

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One of the promising approaches for treatment of diseases and injuries of the skeletal system are tissue scaffolds that combine the ability to support bone tissue regeneration with adequate mechanical strength. Carbon fibers (CFs) are promising candidates for such materials, owing to properties such as low density, electrical conductivity and radiolucency[1-2].

The aim of the study was to charactarize carbon fiber nonwovens produced by carbonization of short, chopped polyacylonitrile fibers. The fibers were oxidized and then functionalized by the electrophoretic deposition (EPD) of hydroxyapatite onto their surfaces. The effects of applied voltage and depostion time on the material's structural organization, fiber diameter, and the adhesion of osteoblastic cells to the fiber surfaces were investigated.

The results indicated that the deposition of hydroxyapatite increased the crystallinity of the nonwovens. Increasing the voltage led to a higher crystalline content in the analyzed materials. The largest fiber diameter was observed in the nonwoven produced as a result of the longest depostion time. Raman spectra obtained after modification revealed a shift in the D1 band position toward higher wavenumbers; this shift may be attributed to interactions between electron-donating aromatic rings in the graphite layers and the electron-accepting P—OH groups in the hydroxyapatite[3-4]. Osteoblastic cells adhered to the surface of the fibers and changes in the G-band position and the value of the R1 parameter was observed[5-6].

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Distance-Dependent Interfacial Coupling in CNT/WSe_2 mixed-dimensional Heterostructures

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Heterostructures with mixed dimensions provide a platform for studying optical interactions across interfaces [1,2]. In this work, we investigate optical coupling at the interface between a single layer of WSe_2 and single-walled carbon nanotubes (6,5). To investigate the effect of the interlayer distance on optical interactions, the phase boundary was modified using hBN layers with thicknesses of 4, 10, and 16 nm.

Resonance Raman spectroscopy was used in this study, revealing changes in the resonances of both the carbon nanotubes and WSe_2 upon formation of the heterostructure, indicating interfacial coupling. Photoluminescence excitation measurements also show an excitation-energy-dependent optical response that differs from that observed in isolated WSe_2. Importantly, the photoluminescence response varies systematically with the distance between WSe_2 and the carbon nanotubes.These results reveal distance- and excitation energy-dependent optical coupling in CNT/WSe_2 heterostructures and demonstrate the potential of nano-scale interface engineering for controlling optical interactions at 1D/2D interfaces.

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Strain-Induced Optical and Electrical Properties of BN Integrated with GaN NWs

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Epitaxial, layered boron nitride is a wide-bandgap material of interest for deep ultraviolet (DUV) and visible optoelectronics due to its high emission efficiency. However, inefficient doping strongly limits successful carrier injection and electroluminescence in this material. To overcome this challenge, approaches based on local structural modification and tunnelling-assisted charge injection have been proposed, enabling carrier transport without conventional bulk doping [1]. Furthermore, local strain has been reported to activate single-photon emission centres and enable light emission [2], motivating studies on strain engineering in BN-based systems.

In this work, we investigate epitaxial BN integrated with GaN nanowires (NWs), focusing on the influence of nanoscale strain induced by the NWs on the optical properties and charge injection mechanism in BN. Epitaxial BN layers were grown by metal-organic vapor-phase epitaxy (MOVPE) on sapphire substrates [3]. To introduce controlled nanoscale strain, the BN layers were transferred onto GaN NWs grown on n-type Si (111) substrates [4].

Raman spectroscopy revealed strain-induced shifts of BN phonon modes. SEM measurements confirmed the surface morphology to be correlated with the nanowire distribution, while AFM studies indicated local deformations in BN layers with thickness below 30 nm. Cathodoluminescence measurements were performed for both BN/Si and BN/GaN NW structures to compare their emission properties and isolate strain-related effects.

To investigate the vertical charge carrier transport, current-voltage measurements were performed on Si (111)/GaN NWs/BN/Au junctions. The obtained characteristics revealed a nonlinear increase in current with a pronounced onset at approximately +9 V (see Fig. 1). Such behaviour is indicative of tunnelling-dominated charge transport and is consistent with the Fowler-Nordheim tunnelling mechanism. These results provide insight into strain- and field-induced phenomena in GaN NWs/BN heterostructures and highlight their potential for novel light-emitting and tunnelling devices.

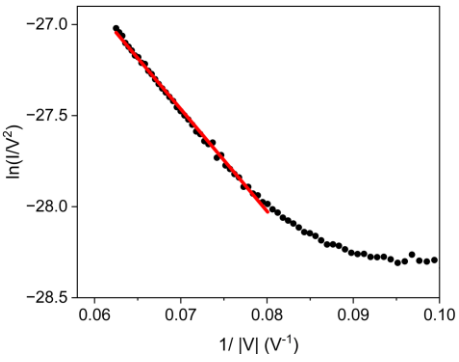


Figure 1. Experimental data (black dots) together with the linear fit (red line) of the Fowler–Nordheim plot for voltages above 11 V.

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Acknowledgments

Project partly founded by Polish National Science Centre grants 2022/04/Y/ST7/00043 (Weave-Unisono), 2021/43/D/ST7/01936 and 2022/45/B/ST5/0287

Isotopic Effects in Epitaxial hBN: Distinguishing Hydrogen-Related Defect Complexes

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Hexagonal boron nitride (hBN) is a layered, wide-bandgap 2D material that has emerged as an excellent host for optically active spin defects [1]. Notably, the negatively charged boron vacancy V_B^- features an S=1 spin state, enabling precise electric and magnetic field sensing in novel quantum sensors. Practical applications require flexible, large-area films, which can be effectively grown via Metal-Organic Vapor Phase Epitaxy (MOVPE) [2]. However, MOVPE growth often introduces complexes of defects rather than isolated vacancies [3]. These are usually accompanied by hydrogen atoms, which reduce the efficiency of spin-active V_B^- centers. A key strategy of detaching hydrogen atoms from these complexes is high-temperature annealing in neutral atmosphere.

In this study, we investigated natural and isotopically enriched ^{10}BN samples grown on 2-inch sapphire substrates via the MOVPE method, which contain a significant amount of vacancy complexes. These materials were analyzed using infrared optical absorption. Comparative measurements between natural BN (^{nat}BN) and ^{10}BN reveal vibrational modes around 3200 cm^{-1} that exhibit an isotopic shift (Fig. 1a), indicating boron atom involvement in the defect complex. Conversely, other hydrogen-related modes (e.g. 3430 cm^{-1}) lack this isotopic effect, suggesting they do not involve boron and may instead relate to boron vacancies (Fig. 1b). To understand their exact nature, we compared as-grown samples with those annealed in nitrogen atmosphere at 1400°C. Finally, temperature-dependent optical absorption measurements reveal mode energy shifts, providing insight into the defects' vibrational symmetry and origin. These results are essential for advancing large-area, MOVPE-grown hBN for quantum sensing.

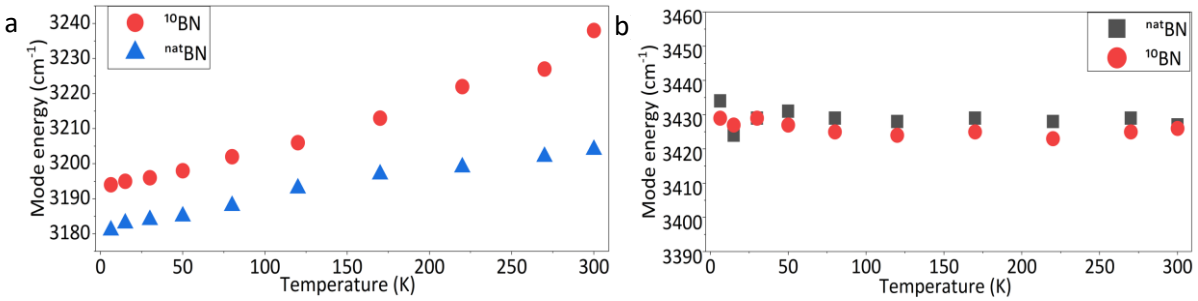


Figure 1. Energy of vibronic modes observed around a) 3200 cm^{-1} and b) 3430 cm^{-1} for natural BN and isotopically enriched layers, measured in the range of temperatures 6 – 300 K.

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This work was supported by the National Science Centre, Poland, under the decision 2022/47/B/ST5/03314.

Towards resonant energy transfer in a $MoSe_2/ReS_2$ 2D heterostructure with tunable interlayer separation

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We present an experimental platform designed to study distance-dependent Förster resonant energy transfer [1] in a $MoSe_2/ReS_2$ van der Waals heterostructure with dynamically controlled interlayer separation. The interlayer distance is tuned in a controlled manner from hundreds to tens of nanometers by piezoelectric positioners, allowing systematic investigation of how photoluminescence (PL) intensity evolves as a function of separation.

The choice of $MoSe_2$ and ReS_2 is motivated by their spectral overlap of $MoSe_2$ absorption and ReS_2 emission (20.7%), which enhances resonant energy transfer between the donor ReS_2 and acceptor $MoSe_2$ layers [2].

The key feature of this approach is the use of piezoelectric positioners to set and adjust interlayer distance between monolayer flakes mounted separately. The approach is conceptually similar to distance control in tunable Fabry-Pérot microcavities, where piezoelectric positioners are used to stabilize and scan the cavity length. This configuration eliminates uncertainties inherent to permanently stacked heterostructures and allows direct experimental access to study coupling mechanisms in a fully tunable geometry. The interlayer distance can be monitored through interference fringes in white light spectrum.

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Thursday 17.9.2026

MBE-grown $PtSe_2$ films for thermal investigations

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This talk presents a selection of reseach activities on molecular-beam-epitaxy (MBE)-grown platinum diselenide ($PtSe_2$) developed at Thales Research & Technology, from material growth and intrinsic thermal properties to applications in power-device thermometry. $PtSe_2$ is a transition metal dichalcogenide whose band structure evolves from semiconducting in the few-layer regime to semimetallic in thicker films, resulting in high electrical conductivity and intermediate in-plane thermal conductivity making it attractive for thermal sensing applications respectively [1,2].

In the first part, I will introduce MBE growth of $PtSe_2$ on sapphire and show how Raman spectroscopy provides fast, non-destructive metrics for film quality. In particular, the full width at half maximum (FWHM) of the in-plane Eg and out-of-plane A1g modes will be discussed as quantitative indicators that correlate with crystalline order and sheet conductance, enabling practical feedback for process optimization [1].

The second part will be dedicated to the intrinsic in-plane thermal conductivity of $PtSe_2$, based on the recent work of Jolivet *et al.* on suspended membranes of MBE-grown $PtSe_2$ [2]. I will briefly describe the semi-dry transfer process used to fabricate multiple suspended membranes from large-area epitaxial films, and then present optothermal Raman measurements where the Raman laser acts as both local heater and thermometer.

In the final part, I will discuss how atomically thin 2D materials such as $PtSe_2$ can be used as nanoscale temperature probes on wide-bandgap power devices [3]. Based on the work from *Carisetti et al.*, here $PtSe_2$ patches, either transferred or grown and patterned directly on metallized surfaces, serve as Raman-active thermometers on a calibrated gold serpentine resistor and on a SiC junction-barrier Schottky diode. The close agreement between techniques on the resistor and the observed impact of the integration route on the SiC device highlight both the potential and the processing challenges of 2D-based Raman thermometry for realistic power electronics.

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Measuring Thermal Properties of 2D Materials and vdW Heterostructures

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Thermal properties are essential for understanding heat transport in two-dimensional (2D) materials and for their integration into next-generation nanoelectronic, optoelectronic, and thermoelectric devices. As the interest in 2D materials and van der Waals heterostructures continues to grow, accurate and reliable characterization of their thermal properties has become increasingly important. However, thermal measurements of atomically thin materials remain challenging because of their small dimensions, complex interfaces, and sensitivity to sample quality and experimental conditions.

In this talk, I will present and compare several experimental techniques used to characterize the thermal properties of 2D materials and van der Waals heterostructures. The presentation will focus on optical methods, including optothermal Raman thermometry[1], frequency-domain thermoreflectance (FDTR) [2], and the combination of Raman spectroscopy with electrical measurements (Fig. 1). The principles, advantages, and limitations of each technique will be discussed, together with recent results on the thermal conductivity and thermal boundary conductance of transition metal dichalcogenide (TMD) samples. Finally, I will compare the capabilities of these methods and discuss their suitability for different classes of materials and device architectures, highlighting recent advances that improve the accuracy and reliability of thermal property measurements.

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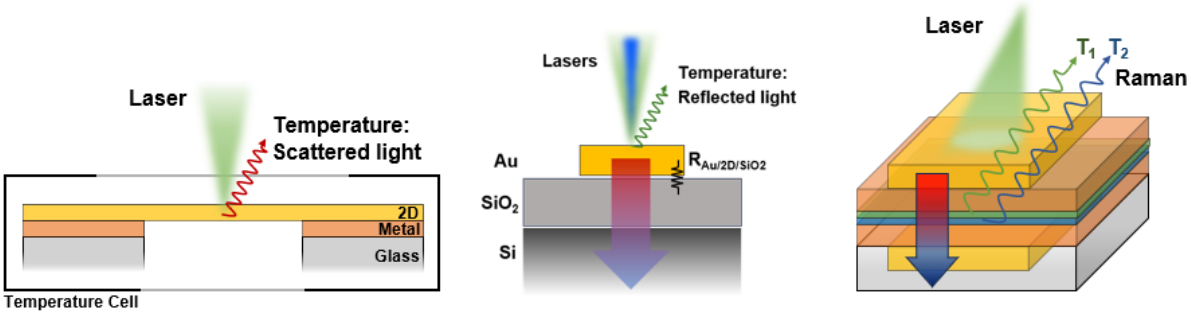


Figure 1. Schematic representation of various measurement techniques.

Molecular beam epitaxy of optically active indium telluride/indium selenide van der Waals heterostructures

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Two-dimensional (2D) crystals, characterized by weak interlayer van der Waals forces and strong in-plane covalent bonds, became one of the leading topics in the condensed matter physics. Stacking two or more such materials on top of each other, forming co called van der Waals heterostructures, significantly broadens the range of observable physical phenomena and enables novel functionalities. The exfoliation technique, commonly used for fabricating van der Waals heterostructures, despite of its scientific importance is inherently limited by the random in-plane sizes of individual 2D flakes, which results in poor scalability of this approach. In contrast, epitaxial technologies, such as molecular beam epitaxy (MBE) used in this work, enable the growth of heterostructures on large, wafer-scale substrates and allow stacking multiple layers in a controlled manner, making it possible to fabricate unique multi-layer heterostructures, such as quantum wells or superlattices.

The aim of this work is the fabrication and optical investigation of novel heteroepitaxial quantum structures composed of indium telluride and indium selenide. For this purpose, we employ our recent finding: the MBE growth of high quality γ-InSe, a semiconductor belonging to the family of 2D materials, on conventional (111)B-GaAs substrate. Using γ-InSe/GaAs as the substrate, InTe/InSe quantum wells are fabricated on wafer-scale areas. Importantly, it is demonstrated that very thin InTe layers within γ-InSe matrix are optically active and that the optical emission energy scales with InTe thickness. More precisely, it can be varied in the near infrared spectral range, from 0.9 eV to 1.3 eV (at 10 K), which is explained by an important contribution of the quantum size effect. These hetrostructures are optimized furthermore to achieve the most intense optical. It is found that the thinnest InTe quantum wells with the emission energy in the range 1.0 - 1.1 eV are characterized by the most intense optical emission. In the case of thicker quantum wells InTe/InSe lattice mismatch and related misfit dislocations result, most likely, in the deterioration of the optical performance

[1] P. Wojnar et al., Quantum Size Effect in Optically Active Indium Selenide Crystal Phase Heterostructures Grown by Molecular Beam Epitaxy, Adv. Opt. Mater. 13, e00738 (2025)

This work has been partially supported by the National Centre of Science (Poland) through grant 2021/41/B/ST3/03651, and by the Foundation for Polish Science project "MagTop" no. FENG.02.01-IP.05-0028/23 co-financed by the European Union from the funds of Priority 2 of the European Funds for a Smart Econom y Program 2021–2027 (FENG).

Facile synthesis of two-dimensional amorphous carbon for enhanced corrosion resistance

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Monolayer amorphous carbon (aC) is a prototype two-dimensional amorphous material with a disordered structure that exhibits significantly lower electrical conductivity than graphene, effectively rendering it an insulator [1,2]. While aC has vast potential for applications such as diffusion barriers, low-*k* dielectrics, and corrosion protection, current synthesis methods often require complex setups or specialized precursors. This work presents an extremely facile, reproducible, and low-temperature (down to 450 °C) chemical vapor deposition method to synthesize MAC on copper using an unconventional carbon source. Through systematic testing, we improve the reproducibility of growth using cost-effective mitigation strategies, such as air- or hydrogen-baking prior to growth. The resulting MAC layers are mechanically robust, wrinkle-free, approximately 1 nm thick, and demonstrate excellent performance as corrosion- and oxidation-protection barriers.

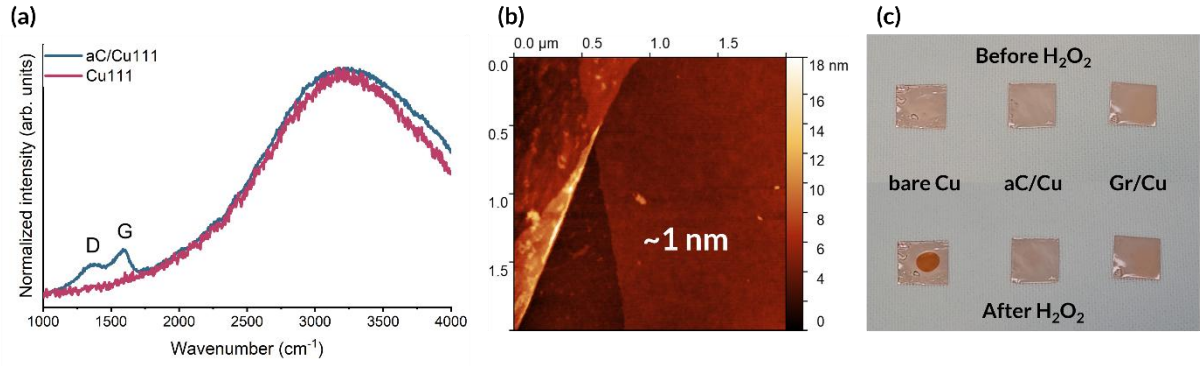


Figure 1. (a) Raman spectrum of aC on copper; (b) AFM of the transferred aC showing 1 nm thickness; (c) optical images of bare copper, copper with aC, and copper with graphene showing excellent oxidation protection of aC.

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Single-molecule chirality: can it be identified?

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Chirality is an intrinsically three-dimensional molecular property, whereas scanning tunneling microscopy (STM) provides an electronic-structure-dependent image of molecules adsorbed on a surface. This raises a fundamental question: **can the absolute handedness of an individual molecule be reliably identified**?

We address this question through studies of [5]- and [7]thiaheterohelicenes and their derivatives on metallic surfaces using STM, tip-enhanced Raman spectroscopy (TERS), STM-induced light emission, and theoretical modelling [1–8]. For racemic 2,13-bis(aldehyde)-[7]thiaheterohelicene on Au(111), high-resolution STM reveals asymmetric intramolecular contrast associated with P and M helicities, enabling heterochiral and locally homochiral arrangements to be distinguished [2]. For racemic [5]thiaheterohelicene on Ag(111), crescent-shaped submolecular features allow the absolute handedness of individual molecules to be identified [4]. However, [7]thiaheterohelicene on Ag(111) illustrates an important limitation: nearly symmetric STM protrusions make direct chirality discrimination difficult [4]. DFT calculations and molecular dynamics simulations instead identify heterochiral dimers as building blocks of zigzag chains [5]. Functionalization strongly modifies chiral recognition. Enantiopure (M)-2,13-diphenyl[7]thiaheterohelicene forms a distorted hexagonal structure on Ag(111), reflecting the interplay between molecule–substrate and intermolecular interactions [6]. Racemic and enantiopure hydroxymethyl-substituted derivatives form apparently similar zigzag chains, although van der Waals interactions dominate in the heterochiral system and hydrogen bonding in the homochiral system [7]. For shorter [5]thiaheterohelicene, substrate registry can dominate over intermolecular chiral recognition [8]. TERS provides nanoscale chemical information but can also perturb molecules, as demonstrated by tip-induced dehydrogenation [1].

These results provide a qualified answer: **single-molecule chirality can be identified when submolecular contrast can be correlated with a well-defined molecular geometry. Otherwise, reliable assignment may require complementary spectroscopy, theoretical modelling, or higher-resolution structural probes**. Thus, molecular chirality is not a universal STM observable, but can become accessible under controlled conditions.

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GRANAD: A tight-binding framework for light-matter interactions and its application to mode-selective spontaneous emission

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Modern nanophotonic design demands specialized theoretical tools capable of capturing light-matter interactions at the atomic scale, where discrete electronic structures govern optical behavior. In this work, we present the formalism and numerical capabilities of GRANAD (GRAphene Nanoflakes with ADatoms), an open-source tight-binding simulation utility designed to model optical and electronic dynamics in nanostructured systems [1].

While the distinction between collective (plasmonic) and single-particle (quantum) resonances in nanostructures is well known, their actual impact on spontaneous emission remains an open question. To examine this relationship and gain intuitive control over the excitation of specific electronic modes, we investigate a point-dipole emitter near a one-dimensional Su-Schrieffer-Heeger (SSH) atomic chain as a benchmark toy model. We analyze how key interaction parameters dictate mode-selective excitations and shape spontaneous emission patterns. This toy-model approach establishes a general framework for mode control that can be applied to more complex two-dimensional nanostructures.

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Supported by the NSC, Poland; project no. 2024/55/D/ST3/02384

Effect of strain and electric field on charge density wave orderings in monolayer tantalum dichalcogenides: a first-principles study

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Tantalum dichalcogenides constitute a particularly interesting subgroup of transition metal dichalcogenides owing to the emergence of charge density wave (CDW) orderings related to lattice distortions in these van der Waals materials [1]. This phenomenon makes them an attractive playground for fundamental physics and enhances their potential for applications. In particular, the T polymorphs of TaS_2 and $TaSe_2$ are known to form a $\sqrt{13} \times \sqrt{13}$ superstructure accompanied by the formation of a CDW, which is robust even at room temperature. Furthermore, CDW ordering can be controlled by a variety of stimuli, such as temperature, electric field, doping, laser illumination, or strain.

In this paper, we discuss the influence of biaxial strain on the CDW-related properties of monolayer tantalum dichalcogenides such as TaS_2 and $TaSe_2$ [2], as well as a Janus-type system, TaSSe [3]. The computational study is based on a first-principles approach. We analyse structural quantities such as interatomic distances, as well as the total energies of the distorted (commensurate CDW) and undistorted (normal) phases, to assess the behaviour of the lattice distortion. We then investigate the charge transfer between atoms in the supercell to shed light on charge-density-related features. To complete the physical picture, we analyse the electronic structure of the systems under consideration.

We find that compressive strain stabilizes the CDW ordering by increasing its energetic stability and enhancing both relative distortion and charge transfer values. In contrast, tensile strain promotes the normal (undistorted) phase. The critical values of tensile strain required to induce switching between the CDW and normal phase are determined.

To gain further insight, we also investigate the influence of an external electric field applied perpendicular to the monolayers on CDW stability, finding pronounced robustness of the CDW phase against this perturbation.

The results may be relevant to understanding the effect of substrates on CDW properties in tantalum dichalcogenides. Moreover, they may aid the design of van der Waals heterostructures with spintronic functionalites involving such materials [4].

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We gratefully acknowledge Polish high-performance computing infrastructure PLGrid (HPC Center: ACK Cyfronet AGH) for providing computer facilities and support within computational grant no. PLG/2025/018673.

Theoretical studies of plasmon and external magnetic field effects on high-harmonic generation in graphene and transition metal carbides and nitrides

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High-harmonic generation (HHG) in condensed matter systems has become intensively studied topic, both, as a source of fundamental insight into phenomena of light-matter interaction, and also as possibility to realize novel light sources in particular energy range, especially to effectively generate high order harmonics in THz spectral range. The two-dimensional (2D) materials have been considered to be promising candidates for systems exhibiting such nonlinear optical phenomena. Some time ago it has been demonstrated that HHG in graphene can be enhanced by utilizing local plasmons in doped graphene nano-structures [1]. Only recently it has been found out that the application of the strong magnetic field to graphene structures can increase harmonic conversion efficiency by orders of magnitude [2].

In the present studies we address three research issues: (i) how other emerging 2D materials transition metal carbides and nitrides (MXenes) compete with graphene in HHG generation process, (ii) does coupling of plasmons with magnetic field increases the intensity of the HHG, and (iii) which effects in HHG can be expected by reducing the dimensionality and symmetry of these 2D materials systems, *i.e*., considering ribbons and flakes.

In our theoretical studies, we choose to use Semiconductor Bloch Equations (SBEs) approach [3] that is routinely employed nowadays for investigation of highly nonlinear response in broad class of materials. The SBEs, which describe time dependence of the density matrix, are attractive because they provide a many-body framework that allows for the treatment of dephasing and population decay. It is also fairly easy to include into the BSEs formalism the Berry connections and transition dipole phases (TDPs), which have to be taken into account for systems lacking inversion or time-reversal symmetries. We employ tight-binding (TB) hamiltonian for the description of electronic degrees of freedom. The external magnetic field is included in the TB hamiltonian through the so-called Peierls substitution, where inter-site hoping matrix elements are modified by phase factors dependent on magnetic field. The laser light pulse is described through time dependent vector potential.

The performed numerical computations demonstrate: (i) positive coupling of plasmons and external magnetic field on the strength of the induced higher harmonics, (ii) the MXenes layer systems exhibit pronounces nonlinear effects, and (iii) the geometry (and therefore the symmetry) of flakes modifies the shape of higher-harmonics spectrum.

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Thursday 18.9.2026

Afternoon Session A

Understanding piezoelectricity in epitaxial boron nitride grown by MOVPE

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Significant scientific interest has been attracted to piezoelectricity in two-dimensional materials, since DFT calculations predicted strong in-plane electromechanical coupling in monolayers of transition metal dichalcogenides and boron nitride (BN) [1]. This phenomenon has been experimentally demonstrated for the first time in monolayers of molybdenum disulfide in pioneering papers from 2014 and 2015 [2, 3]. Piezoelectricity in 2D systems can be combined with their exceptional mechanical, optical and electronic properties, paving the way for novel nanodevices. One of the most promising 2D materials is hexagonal boron nitride with different stacking sequences of atomic layers, so-called polytypes, which provide distinct symmetries of crystal structures. As piezoelectric properties are determined by the crystallographic point groups, BN occurs in piezoelectric and non-piezoelectric forms.

In this work, we investigate thin films of epitaxial BN grown using metal-organic vapour phase epitaxy. The local electromechanical response of several samples was characterised using piezoresponse force microscopy (PFM). PFM measurements reveal the coexistence of two types of piezoelectric domains, marked with green and red dots in Fig. 1c), which exhibit similar amplitudes of the piezoelectric response with a 180° phase shift. We will propose a possible stacking-related origin of the phase contrast and compare effective magnitudes of piezoelectricity between different samples, highlighting the explanation of the wide range in piezoelectric response. We will also clarify the origin of vertical piezoelectricity in BN.

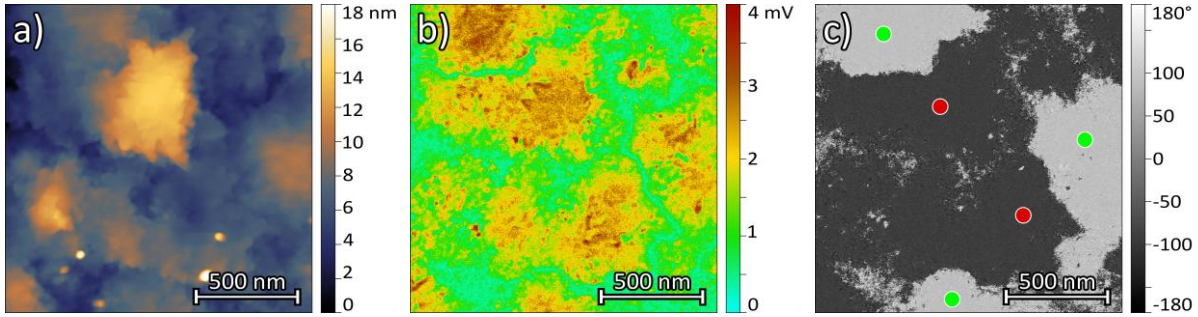


Figure 1. Contact mode topography (a), out-of-plane PFM piezoresponse amplitude (b), and out-of-plane PFM piezoresponse phase (c) – images of epitaxial BN growths.

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Acknowledgments

This research is supported by the Polish National Science Centre grant no. 2022/47/B/ST5/03314.

11th Polish Conference “Graphene and other 2D Materials”

Spatially correlated TEM-AFM-KPFM imaging of BN piezoelectric domains

Izabela Rogala[1], Jan Złotopolski-Pirczewski[1], Jakub Iwański[1], Anna Kaleta[2], Rafał Bożek[1], Jan Pawłowski[1], Marta Bilska[1], Sławomir Kret[2], Johannes Binder[1] and Andrzej Wysmołek[1]

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The properties of two-dimensional (2D) materials are strongly influenced by the stacking sequence of their atomic layers. Depending on the stacking sequence and resulting crystal symmetry, different polytypes may exhibit distinct physical phenomena, including ferroelectricity, piezoelectricity, and second harmonic generation (SHG), arising from the absence of inversion symmetry [1]. Layered boron nitride (BN), a wide-bandgap 2D material, exhibits numerous stacking polytypes. The most extensively studied are the centrosymmetric hexagonal phase (hBN, AA’ stacking) and the noncentrosymmetric rhombohedral (rBN, ABC stacking) and Bernal (bBN, AB stacking) phases [2].

In this work, we investigate BN epitaxial layers grown by metal-organic vapour phase epitaxy (MOVPE), in which multiple polytypes coexist. Kelvin probe force microscopy (KPFM) measurements reveal two types of domains exhibiting different surface potentials. Direct experimental verification of the microscopic origin of such KPFM response remains challenging. Transmission electron microscopy (TEM) of cross-sectional specimens is the most reliable technique for identifying BN polytypes at the atomic scale. However, it probes only a highly localized region of the sample. Consequently, independently performed KPFM and TEM measurements cannot directly correlate the observed surface-potential contrast with the underlying BN polytype. Establishing such a correlation requires locating exactly the same microscopic region during AFM imaging and TEM lamella preparation. Then, within the correlated area, one must locate the narrow line that becomes the final TEM profile after lamella thinning. In this work, we overcome these experimental challenges and demonstrate a direct correlation between KPFM contrast and the atomic structure resolved by TEM. We establish a clear relationship between regions of opposite KPFM potential and specific BN polytypes, as presented in Figure 1. This correlative methodology provides new insight into the direct origin of piezoelectric response in epitaxial BN and offers a valuable tool for the development of BN-based devices exploiting SHG, ferroelectricity, and piezoelectricity.

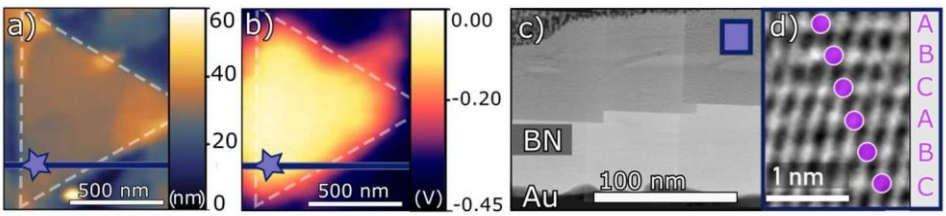


Figure 1. BN polytypic domain characteriza on. a) AFM topography. b) KPFM poten al of the same area, Lines in a) and b) mark the TEM lamella profile. c) TEM cross-sec on image of the area marked with the star. d) HRTEM image of a fragment of image marked by a rectangle in c) showing ABC stacking.

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Second Harmonic Generation Induced UV Luminescence in Rhombohedral Boron Nitride Films

Bazlul Karim,[1] Krzysztof P. Korona[2], Aleksandra K. Dąbrowska[2], Mateusz Tokarczyk[2], Jakub Iwański[2], Johannes Binder[2], Andrzej Wysmołek[2], and Mariusz Klimczak[2]

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Defect-induced photoluminescence (PL) in sp^2-bonded layered boron nitride (BN) at 4.1 eV (C300), originating from carbon-dimer defects (C_BC_N), has been extensively investigated in recent years because of its bright emission, high single-photon purity [1], and utility in differentiating sp^2-BN polytypes, which arise from different stacking arrangements of the 2D atomic planes [2]. This work demonstrates that such structural polytypism can give rise to distinct optical nonlinearities in hexagonal and rhombohedral BN films, studied here on MOVPE-grown samples, by altering the crystal symmetry, and induce the characteristic 4.1 eV PL emission via the up-conversion of sub-4.1 eV photons through two-photon absorption (TPA) and second-harmonic generation (SHG), respectively. The spectral features of this PL are similar to those obtained under single-photon excitation (SPX). A comparative analysis, however, revealed that SHG in non-centrosymmetric rhombohedral BN provides a more efficient optical excitation pathway to activate the C300 PL emission using much lower-energy photons, owing to its high second-order electrical susceptibility [20(7) pm/V]. Our findings thus emphasize that polytypism is an attractive tool for designing up-conversion-driven defect luminescence in sp^2-bonded BN across a wide spectral range, including deep-UV, opening possibilities for the development of diverse quantum photonic technologies [3].

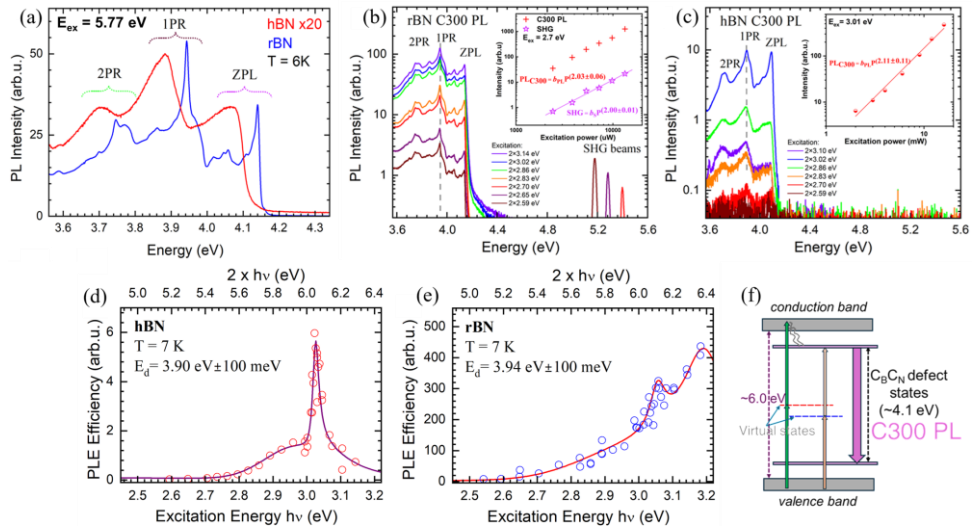


Figure 1. (a)-(c) C300 PL at 4.1 eV in MOVPE-grown sp^2-bonded BNs under SPX (a) and sub-4.1 eV excitations (b) & (c). (d)-(e) Photoluminescence excitation spectra of C300 defect luminescence in hBN and rBN, respectively. (f) A schematic illustrating the up-conversion-induced optical transitions in sp^2-bonded BNs leading to C300 PL.

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Acknowledgement

This research was supported in the scope of NCN OPUS UMO-2023/51/B/ST7/01204.

Local Formation of Resistive States in Ultrathin α-MoO_3

Aleksandra Nadolska[1], Iaroslav Lutsyk[1], Michał Piskorski[1], Paweł Krukowski[1], Paweł Dąbrowski[1], Witold Kozłowski[1], Paweł J. Kowalczyk[1], Maciej Rogala[1]

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Resistive switching in ultrathin oxide layers involves electrically induced changes in local conductivity and charge transport. When the active material is reduced to a few atomic layers, the electrical response becomes highly sensitive to thickness, stoichiometry, surface morphology, and the local concentration of defects. This makes atomically thin oxides a suitable platform for investigating resistive switching at the nanoscale without relying on device-averaged measurements.

Here, we investigate local resistance-state formation in crystalline MoO_{3-x} films ranging from a monolayer to several atomic layers. The films were grown by thermal evaporation under ultra-high vacuum conditions on highly oriented pyrolytic graphite. X-ray photoelectron spectroscopy reveals slight oxygen deficiency, particularly in the monolayer regime, where reduced Mo species indicate vacancy-related defects.

Conductive atomic force microscopy was used to map the local current distribution and perform voltage stimulation with a conductive probe. Local current-voltage measurements show bipolar resistive switching, with SET transitions occurring under negative bias and RESET transitions under positive bias. The switching response depends on film thickness, indicating that the number of layers and defect distribution influence the local electrical behavior. Repeated stimulation can also induce irreversible local modifications, suggesting electric-field-driven defect generation, redistribution, or structural degradation. These results show that ultrathin MoO_{3-x} films support local formation of resistance states, making them a useful model system for studying defect-assisted resistive switching in two-dimensional transition metal oxides.

Acknowledgments

This work was supported by the National Science Centre, Poland, under the Grant 2020/38/E/ST3/00293.

Resonant enhancement of second harmonic generation in rBN metasurfaces

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Rhombohedral boron nitride (rBN) is a two-dimensional wide-bandgap semiconductor that shares the in-plane structure of hexagonal boron nitride, but adopts an ABC stacking sequence. This configuration breaks inversion symmetry and thus permits second-order nonlinear optical processes, in particular second harmonic generation (SHG).

Here we use finite-difference time-domain simulations to design an rBN metasurface consisting of a square periodic array of holes (Fig. 1a). Similar photonic structures have been shown to strongly enhance SHG relative to bulk material [1]. Furthermore, the array's geometric parameters are chosen such that the second harmonic is aligned to a carbon-related colour centre with the zero-phonon line near 380 nm [2].

A resonance mode at the primary wavelength, associated with a sharp decrease in transmission, may amplify the second harmonic conversion efficiency, yielding SHG enhancement of up to six orders of magnitude within a narrow spectral window (Fig. 1b). This enhancement grows with the nonlinear material thickness, up to about 80 nm (Fig. 1c). Increasing the thickness also coincides with a redshift of the resonance. The resonance wavelength can be further tuned through the lattice spacing (increasing leads to a redshift) and the hole diameter (blueshift). A metasurface with 80 nm thickness, 500 nm spacing and 223 nm diameter is predicted to yield peak SHG enhancement by a factor of 7630 at 377 nm, providing a concrete target for fabrication and characterization.

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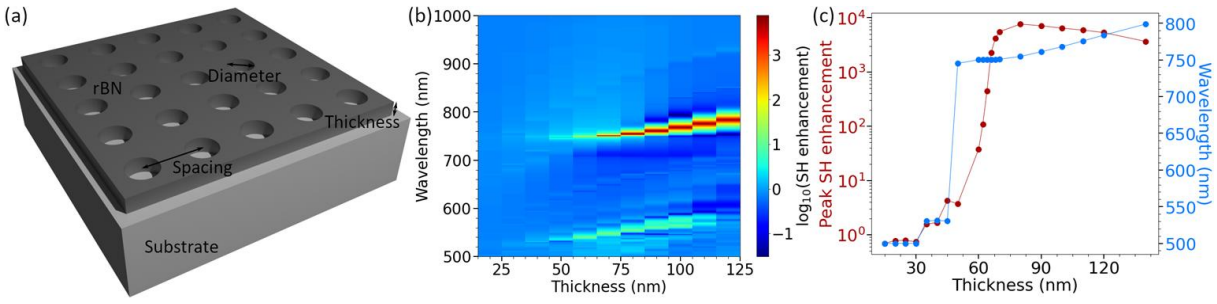


Figure 1. (a) Illustration of the simulated metasurface. (b) SHG enhancement versus nonlinear material thickness and wavelength (spacing 500 nm, diameter 223 nm). (c) Peak SHG enhancement (red) and the corresponding resonance wavelength (blue) versus layer thickness.

Substrate dependent properties of epitaxial BN heterostructures

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The continuous search for more efficient deep-ultraviolet (DUV) light sources has drawn significant attention to hexagonal boron nitride (h-BN), a wide-bandgap semiconductor capable of emitting light at wavelengths as short as 210 nm [1]. In addition to its intrinsic DUV emission, h-BN can host deep defect states within its bandgap. When properly controlled, these defect centres may act as room-temperature single-photon emitters [2], opening new opportunities for applications in quantum photonics. DUV technologies based on AlGaN quantum wells and mercury lamps are limited by low efficiency and poor integration, respectively, motivating alternative platforms such as van der Waals (vdW) heterostructures. In this work, we investigate vdW heterostructures composed of few-layer graphene (FLG) electrodes and epitaxially grown BN layers (15 to 45 nm) [3], with representative I-V curve shown in Fig. 1. The structures were fabricated on both conventional Si/SiO_2 and sapphire substrates to assess the influence of the substrate on device performance. In particular, we compare the electrical characteristics of silicon- and sapphire-based devices, with emphasis on leakage currents, parasitic conductive channels, operating voltages, and device reliability. The fabricated structures withstand electric fields of up to 0.7 V/nm. This study focuses on evaluating the functionality and key performance parameters of BN-based vdW heterostructures and on identifying substrate-dependent factors that may enable the development of efficient DUV emitters and quantum photonic devices. The use of epitaxial material provides a novel route towards scalable tunnelling heterostructures, offering promising prospects for DUV light-emitting devices and electrically driven single-photon emitters.

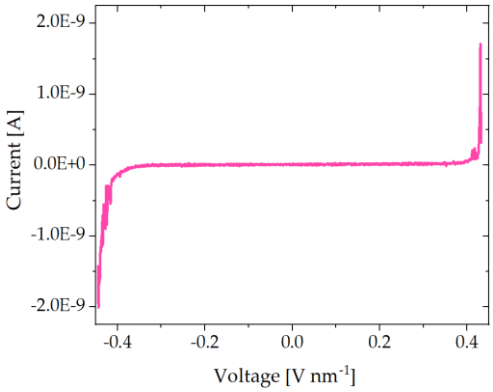


Figure 1. I-V characteristics of tunneling heterostructure FLG/BN epilayer (45 nm) on sapphire substrate.

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Acknowledgments

The authors acknowledge financial support from NCN under Grant 2024/54/E/ST7/00273.

Pristine 2D Interfaces: Eliminating Contamination via Mechanical Sweeping

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Two-dimensional materials and their heterostructures hold immense potential for next-generation materials science and optoelectronics due to their atomically thin nature and tunable properties. However, transfer-induced impurities, residues, and interfacial bubbles severely degrade electrical, optical, and mechanical performance [1]. While AFM probe contact-mode nano-ironing offers in situ cleaning with real-time nanoscale observation, scaling to large-area fabrication remains challenging. We report a scalable fabrication method combining Au-assisted exfoliation for millimeter-scale monolayer extraction [2] with optimized nano-ironing to eliminate transfer bubbles and impurities in 2D homobilayers and heterobilayers (WSe_2/MoS_2). This hybrid mechanical protocol achieves 100% bubble-free interfaces across 10×10 μm² areas (Figure 1), outperforming thermal annealing and plasma methods that risk lattice damage. The AFM cleaning was performed in contact mode at 1Hz, 1024 scan lines, deflection set point 8.11 nm and a force of 200nN. The 200nN force is the bare minimum to clean the HS. Force less than 200 nN requires multiple scans and results are not promising too.

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Acknowledgments

The research was funded by the Warsaw University of Technology within the Excellence Initiative: Research University (IDUB) programme

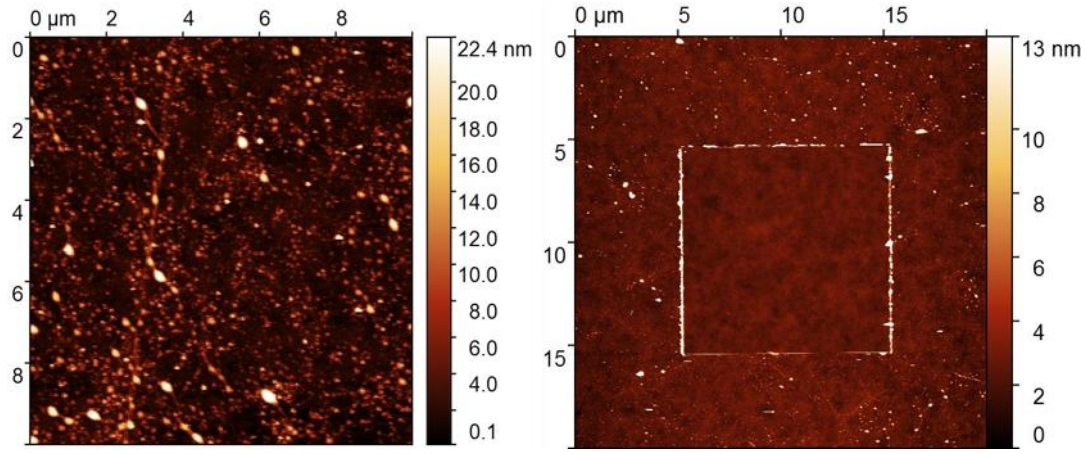


Figure 1. AFM analysis of Hetero bi-layers. (a) Before AFM tip cleaning (b) After AFM tip cleaning

Field induced polarization enhancement in TMD monolayer as a sensitive probe of magnetic effects in 2D heterostructures

Wojciech Kolesiński,[1] Maksymilian Kuna[1] , Tomasz Kazimierczuk[1] , Takashi Taniguchi[2], Kenji Watanabe[2], Piotr Kossacki[1] , Mateusz Goryca [1]

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When magnetic and non-magnetic materials are brought into close proximity, the magnetic order of the former can significantly influence the physical properties of the latter[1]. This interaction becomes particularly pronounced in atomically thin van der Waals heterostructures, where the extremely small thickness and atomically sharp interfaces enhance interlayer coupling.

As a platform to investigate this phenomenon, we employ a $CrSiTe_3/WSe_2$/hBN heterostructure. $CrSiTe_3$ is a layered ferromagnetic material characterized by low coercivity and a relatively low Curie temperature. In contrast, monolayer WSe_2 is a direct band-gap semiconductor with well-understood optical and excitonic properties. One notable feature of WSe_2 is the spin–valley locking that distinguishes electronic states in different valleys of the Brillouin zone. This property enables selective excitation of carriers in each valley using circularly polarized light. However, these valley states experience rapid spin relaxation, resulting in a very low degree of polarization of photoluminescence associated with delocalized excitonic states. In the case of localized states, however, this relaxation can be strongly suppressed by even a small external magnetic field, leading to a phenomenon known as field induced polarization enhancement[2].

In this work, we use this enhancement as a sensitive probe of the presence of the magnetic proximity effect. Thanks to sample's design, photoluminescence can be measured in both hBN/WSe_2/$CrSiTe_3$ and hBN/WSe_2 heterostructures within the same sample. Consequently, the two signals can be compared under identical experimental conditions, minimizing the influence of external factors that could otherwise affect the results. We measure the degree of polarization as a function of the external magnetic field, as well as the temperature dependence of the polarization enhancement. We observe measurable polarization enhancement even without the external magnetic field in the hBN/WSe_2/$CrSiTe_3$ region, which indicates the presence of the magnetic proximity effect within that structure.

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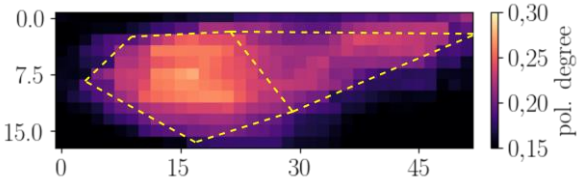


Figure 1. Map of the polarization degree of the sample. hBN/WSe_2/$CrSiTe_3$ on the left and hBN/WSe_2 on the right, measured at 6 K.

Epitaxial boron nitride as a platform for versatile moiré heterostructures - a cathodoluminescence study

B. Furtak[1], A. K. Dąbrowska[1], K. Korona[1], A. Reszka[2], S. Piotrowska[2], B. J. Kowalski[2], J. Binder[1], A. Wysmołek[1]

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Hexagonal boron nitride (h-BN) is a layered wide-bandgap semiconductor (≈6 eV) that has emerged as an attractive material for deep-ultraviolet and visible optoelectronic applications as well as van der Waals heterostructures. Although twist-induced moiré superlattices have been extensively investigated in transition metal dichalcogenides [1] and graphene-based systems [2], their influence on the structural and optical properties of boron nitride remains only sparsely explored.

In this work, we investigate a series of twist-angle h-BN heterostructures fabricated from Metalorganic Vapor Phase Epitaxy (MOVPE)-grown epitaxial layers using cathodoluminescence (CL) measurements. Earlier studies reported a broad luminescence band near 4 eV in exfoliated bulk twist-angle structures [3]; however, the origin of this feature remains under discussion, while the limited control over flake dimensions and thickness hinders reproducibility. These limitations are addressed by employing wafer-scale epitaxial h-BN, enabling the fabrication of numerous heterostructures with controlled twist angles while minimizing sample-to-sample variability.

The CL measurements reveal pronounced twist-angle-dependent modifications of the C2 defect emission, including changes in both spectral profile and intensity that cannot be explained solely by optical interference effects. To further examine this behavior, additional heterostructures were fabricated from layers of different parameters and thoroughly characterized. Particular attention was also devoted to improving the quality of the twisted interfaces by optimizing the transfer process and reducing interfacial contamination, creating near-atomically flat interfaces, thereby allowing the observed optical response to be systematically investigated.

These results demonstrate a versatile platform for studying twist-angle phenomena in epitaxial h-BN and provide strong evidence for moiré-induced modifications of defect-related emission in this material. The epitaxial approach further provides precise control over layer thickness, crystal polytype, and growth-related defect concentration, whereas a dedicated flake-transfer system ensures accurate alignment of the interlayer rotation.

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Thursday 18.9.2026

Afternoon Session B

Graphene encapsulation of FeI_2 monolayer: Induced Modifications of Electronic Structure and Lattice Dynamics

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Two-dimensional magnetic materials have attracted considerable interest because of their potential for next generation spintronic applications. Among them, transition metal dichalcogenides show rich magnetic behavior coming from reduced dimensionality, strong electronic correlations, and spin orbit coupling [1]. When coupled with graphene, these materials form van der Waals heterostructures in which electronic, magnetic, and vibrational properties can be modified by interlayer interactions. In this work, we investigate monolayer FeI_2 encapsulated in graphene, with particular focus on graphene induced changes in its electronic structure and lattice dynamics. Using first principles density functional theory, we analyze how graphene encapsulation and the resulting van der Waals pressure alter the electronic band structure of FeI_2, leading to modifications of its low energy states and magnetic interactions. An effective exchange interaction model is constructed through Wannier interpolation, used for a detailed characterization of the magnetic properties. Lattice dynamic is studied using a supercell based phonon approach showing significant changes in the phonon spectrum induced by graphene encapsulation and interlayer coupling. The role of van der Waals pressure is examined as a key factor governing both electronic and vibrational renormalization. The magnetic hysteretic response of the heterostructure is further analyzed through a decomposition into diamagnetic, paramagnetic, and ferromagnetic contributions, associated with graphene, different nanoparticles and FeI_2 magnetic phases. These results show how graphene encapsulation can be used as an effective way for tuning the electronic, magnetic, and vibrational properties of two-dimensional magnetic materials.

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Torsion-Driven Electronic and Magnetic Phase Transition in Boron Atomic Chains

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Mechanical control of electronic and magnetic phases offers a promising route to reconfigurable functionalities in low-dimensional materials. In this work, we demonstrate that experimentally relevant boron atomic chains exhibit a torsion-driven transition from a metallic spin-polarized phase to a nonmagnetic semiconducting state. Using first-principles calculations, we show that twisting the chain from planar *cis*-B_8 to screw-symmetric *trans*-B_8 opens an indirect band gap of approximately 0.5 eV while completely quenching the magnetic moment (see Fig. 1). Phonon calculations further identify *trans*-B_8 as the dynamically stable ground-state configuration. To clarify the microscopic origin of this transition, we develop an effective tight-binding analysis, which reveals that torsion strongly suppresses the dominant longitudinal hopping channel. This reduction in hopping drives a Peierls-like instability that destabilizes the metallic phase and stabilizes the semiconducting state. Our results establish boron atomic chains as a mechanically programmable platform for electronic and spintronic applications, providing a potential route toward torsion-controlled nanoscale devices [1-3].

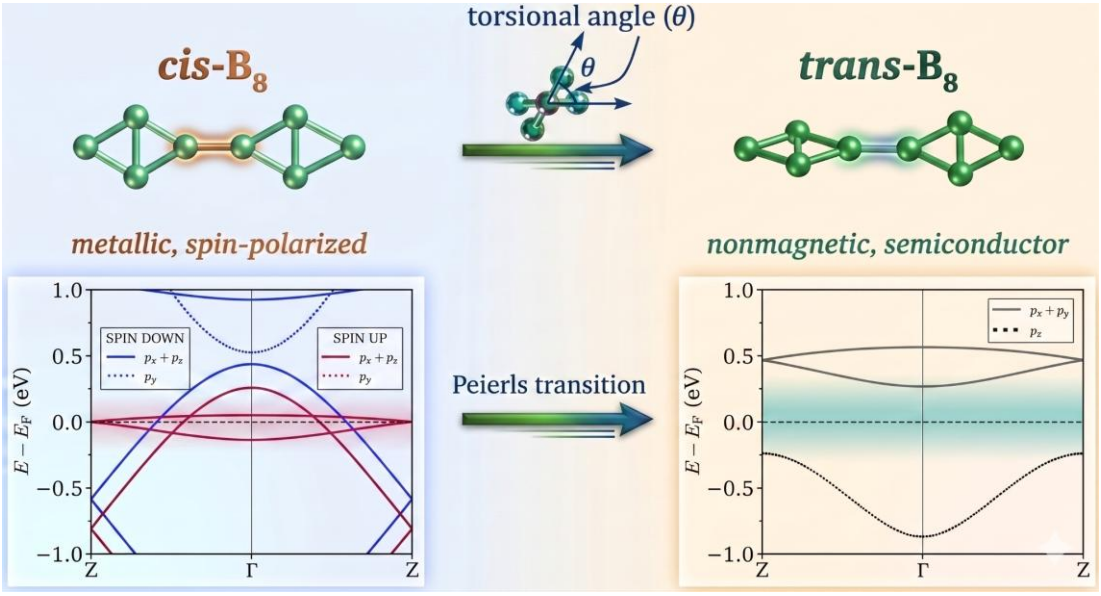


Figure 1. Torsion-driven electronic phase transition in boron atomic chains. The upper panel illustrates the structural transformation from the planar *cis*-B_8 chain (θ = 0°) to the screw-symmetric *trans*-B_8 chain (θ = 90°) through torsional rotation. The lower panels compare the corresponding electronic band structures.

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Acknowledgments

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Superconducting and dielectric properties of monolayer α-$TaSi_2N_4$

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[2]*Institute of Experimental Physics, Slovak Academy of Sciences, Watsonova 47, 04001 Košice, Slovakia*

The monolayer α-$TaSi_2N_4$ belongs to the recently discovered [1] MA_2Z_4 family of two-dimensional layered materials, which exhibit a wide range of tunable physical properties, including semiconducting, metallic, topological, and superconducting phases. The successful synthesis of related compounds, such as $MoSi_2N_4$ and WSi_2N_4, highlights the versatility and technological potential of this class of materials.

In this work, we investigate the superconducting and dielectric properties of monolayer α-$TaSi_2N_4$ using a combination of first-principles calculations and effective tight-binding modeling. The superconducting properties are studied within the framework of Migdal–Eliashberg theory, employing electron–phonon coupling parameters obtained from density functional theory and a Wannier-based Hamiltonian. Our results reveal that α-$TaSi_2N_4$ exhibits anisotropic two-band superconductivity.

The dielectric response is analyzed by evaluating the electronic susceptibility within linear-response theory using the random phase approximation. By combining Green's function techniques with tight-binding modeling, we obtain a microscopic description of the electronic screening and the screened Coulomb interaction. The calculated dielectric screening is subsequently effectively incorporated into the superconducting formalism, allowing us to investigate its influence on the superconducting properties of α-$TaSi_2N_4$, including the superconducting gap structure and critical temperature.

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Acknowledgments:

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PURCELL ENHANCEMENT BY THE EDGE STATES OF ZIG-ZAG GRAPHENE NANOFLAKES

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Graphene nanoflakes with zig-zag edges exhibit distinct and highly localized edge states [1,2] that impart metallic character to the edges, while the interior remains insulating. This pronounced spatial variation in electronic behaviour makes such systems particularly attractive for nanophotonic applications. When a quantum emitter is placed near the flake[3], coupling to these edge states can significantly enhance its spontaneous emission rate, whereas the insulating bulk contributes minimally. These edge states are geometric rather than topological in origin, rendering them sensitive to external perturbations. In this work, we analyse the behaviour of these states across various nanoflake geometries like triangular, hexagonal, and rhombic, focusing on their stability under electron-electron interactions and doping. We find that in the absence of interactions, coupling to edge states consistently enhances the emitter's decay rate. However, the persistence of these edge-induced transitions depends strongly on sublattice symmetry [4]: sublattice-balanced geometries support edge states even under weak interactions, while sublattice-imbalanced structures lose them rapidly. Interestingly, we demonstrate that careful doping can partially restore edge-state transitions in sublattice-imbalanced flakes, offering a pathway to engineer and control light-matter interactions in graphene nanostructures through both geometry and electronic tuning.

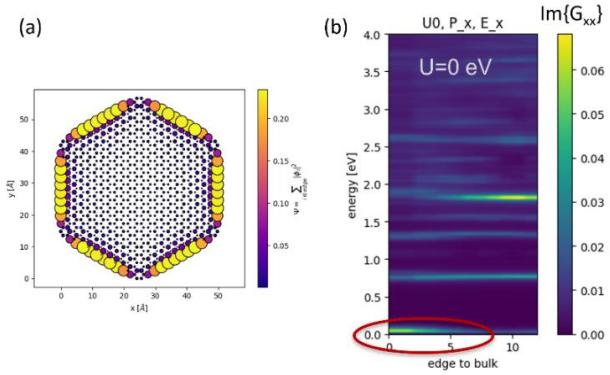


Figure 1: (a) Geometric edge states of a hexagonal zigzag graphene flake. (b) Imaginary part of the scattered Green's function as a function of the quantum emitter's position, from the edge to thebulk.

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Temperature-Dependent Vibrational Properties of Monolayer WS_2 Nanocrystals: From Harmonic Phonons to Ab-Initio Molecular Dynamics

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Two-dimensional transition metal dichalcogenides (TMDCs) exhibit vibrational properties that are highly sensitive to dimensionality, strain, and finite-size effects. While phonons in extended (periodic) monolayer crystals are well understood, less is known about nanoscale TMDC systems like quantum dots and nanocrystals, despite experimental evidence of size-dependent vibrational signatures.[1] In particular, Raman measurements on WS_2 and MoS_2 quantum dots have revealed systematic shifts of characteristic phonon modes with decreasing lateral size, motivating atomistic modelling beyond the extended monolayer limit.[1]

In this work, we investigate vibrational properties of triangular monolayer WS_2 nanocrystals using first-principles calculations, as a function of nanocrystal size, with edge lengths corresponding to 1–10 lattice constants. We observe a gradual convergence of vibrational properties towards the extended monolayer limit, allowing the identification of a characteristic length scale at which finite-size effects become negligible and bulk-like lattice dynamics are recovered. Special attention is given to Raman-active phonon modes, thermal expansion of the nanocrystals, and temperature-dependent anharmonic effects.

The study combines density functional theory (DFT), finite-displacement phonon calculations, the quasi-harmonic approximation (QHA), and ab-initio molecular dynamics (AIMD). While standard harmonic and quasi-harmonic approaches provide a baseline description of lattice dynamics and thermal expansion, AIMD enables a fully anharmonic and explicitly temperature-dependent treatment of vibrational effects in finite systems. This framework allows a critical assessment of the validity of harmonic and quasi-harmonic phonon methodologies when applied to nanoscale two-dimensional crystals at finite temperature.

Our results demonstrate pronounced finite-size effects manifested by shifts and broadening of WS_2 vibrational modes. The AIMD-derived temperature trends reveal clear limitations of the quasi-harmonic approximation in ultrasmall nanocrystals, where anharmonicity and structural fluctuations become dominant. The present work builds upon previous studies of phonon anharmonicity in low-dimensional van der Waals materials and heterostructures[2–5], extending them towards finite-size TMDC nanocrystals. Our data provide a unified atomistic framework for interpreting vibrational properties of nanoscale WS_2.

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Acknowledgments

This research was funded in whole or in part by National Science Centre, Poland (2025/09/X/ST3/00614).

Cross-Plane Thermal Transport in vdW Heterostructures via Joule Heating and Raman Thermometry

Leo Sagan[1], S. H. A. Jaffery[1], K. Wilczyński[1], M. Zdrojek[1], A. P. Gertych[1]

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The growing interest in two-dimensional (2D) materials has stimulated extensive research into their physical properties, yet thermal transport remains insufficiently understood due to the experimental challenges associated with their atomic-scale thickness. While most studies focus on in-plane heat transport, out-of-plane thermal transport is equally important for thermal management in nanoscale electronic and optoelectronic devices, where quantitative measurements of interfacial thermal conductance remain limited.

In this work, we introduce a new Raman-based approach that enables the temperature of each individual layer within a multilayer heterostructure to be measured independently. By resolving the temperature of each constituent material, the proposed method allows the thermal conductance of every interface in the heterostructure to be determined separately. A schematic representation of the measurement principle is shown in Fig. 1.

The method was validated using Al_2O_3, yielding thermal conductance values in good agreement with the literature [1]. It was then applied to hBN/$MoSe_2$/WSe_2, hBN/WSe_2/$MoSe_2$, and hBN/MoS_2/WSe_2 heterostructures to determine the thermal conductance of each interface. In addition, we investigated the external temperature dependence on the interfacial thermal conductance. To the best of our knowledge, such temperature-dependent measurements of individual interfaces in these heterostructures have not been reported previously.

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Acknowledgments

The authors acknowledge financial support from the Polish National Science Centre under the OPUS grant No. 2025/57/B/ST11/02260.

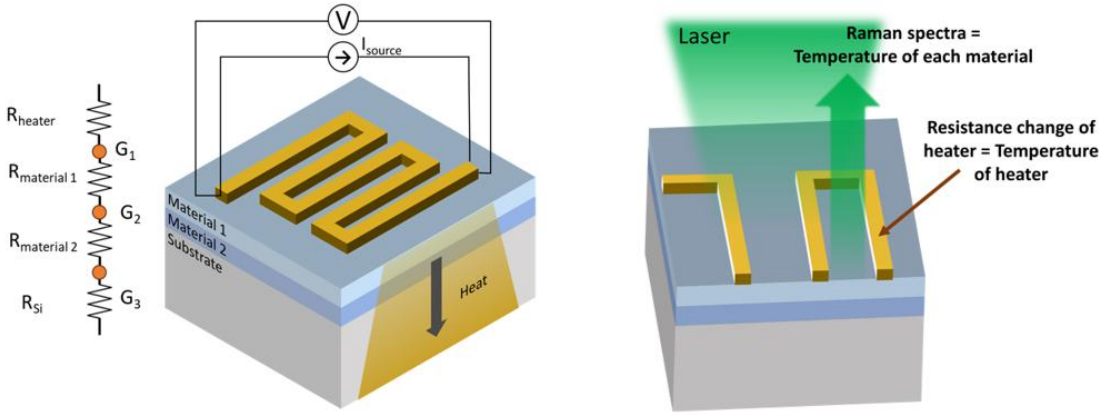


Figure 1. Schematic illustration of the proposed method for measuring the thermal conductance of interfaces in 2D material heterostructures.

Doping of MOVPE-Grown Layered Boron Nitride: Correlation Between Doping Process and Electrical Transport Mechanisms

J. J. Cwynar, A. K. Dąbrowska, K. P. Korona, P. Chyży, M. Tokarczyk,

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As a two-dimensional (2D), ultrawide bandgap (~6 eV) material, layered boron nitride (BN) holds great promise in the field of optoelectronic applications in the deep ultraviolet (DUV) spectral range. However, progress in this area is currently limited due to the ongoing challenge of establishing efficient n-type and p-type doping methods.

In this work, we aim to study the impact of growth parameters on the electrical transport properties of BN doped with silicon. We investigated a variety of procedures in Metal-Organic Vapor Phase Epitaxy (MOVPE) based on pulsed growth mode, which are schematically shown in Fig. 1a. All of the studied samples were also annealed post-growth at 1400°C in a nitrogen atmosphere inside our MOVPE reactor in order to remove hydrogen from the material, which effectively passivates the defects responsible for conductivity [1].

Preliminary results show that there are two transport mechanisms present in the researched doped BN. An exemplary result of temperature-dependent I-V characteristics measurement for sample C(Si) is shown in Fig. 1b. It displays that a simple Arrhenius model is insufficient for the description of that relationship. However, a fitted linear combination of two Arrhenius terms yields activation energies of up to 0.62 eV. Additionally, other transport mechanisms such as variable range hopping might be present. The relevance of the aforementioned processes and how they differ between the samples will be discussed.

Our research addresses the challenge of understanding transport mechanisms in silicon doped BN. It is a great step toward realising boron nitride's potential in DUV optoelectronic devices.

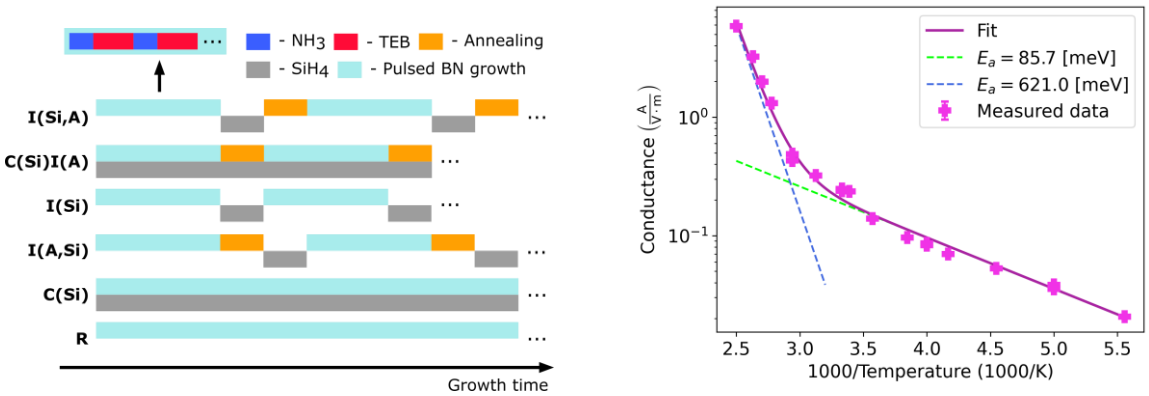


Figure 1. (a) Different samples' growth schematics (b) Relationship between conductance and temperature.

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Acknowledgements

This work has been partially supported by the National Science Centre under grant no. 2024/55/B/ST3/02117

Conductive epitaxial boron nitride: SIMS studies on acceptor activation and electrical properties

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Two-dimensional boron nitride (sp^2-BN) is a very durable insulating material, most commonly employed as a passivation layer. Lately, it has garnered attention due to its efficient light emission in the deep UV range [1] and as a host for bright single-photon-emitting defects [2]. However, accessing the full potential of this material is limited by the lack of efficient doping methods. This study addresses this issue by investigating the electrical properties and composition of both conductive and nonconductive sp^2-BN samples.

The studied sp^2-BN epilayers were grown by Metalorganic Vapor-Phase Epitaxy (MOVPE) on 2-inch sapphire substrates at about 1200 °C. The grown material is nonconductive until annealed in a nitrogen atmosphere at 1400 °C. To examine electrical properties of the conductive material, the layers were fabricated into Hall bars via photolithography. Fig. 1a shows the results of I-V measurements for such a sample, showing ohmic conductivity in the longitudinal direction and only a small, current-independent voltage signal in the transverse direction, indicating high electrical quality for an ultrawide bandgap material.

To examine the compositional changes that activate conductivity, Secondary Ion Mass Spectrometry (SIMS) measurements were performed on sample sets from the same growth process, both as-grown (nonconductive) and annealed (conductive). The results (Fig. 1b,c) show that both samples contain silicon, though the annealed sample exhibits a steep concentration decrease near the surface and a decrease in hydrogen concentration, which we associate with the conductivity activation process. Because the profiles show no clear distinction between the sp^2-BN and substrate signals, drawing meaningful conclusions about the interface is difficult. To resolve this, we delaminated the grown sp^2-BN layer [3] and transferred it onto a new sapphire substrate with a hole (Fig. 1d). The resulting membranes are durable and were able to withstand SIMS measurements, therefore providing a new pathway for measurements on large-area sp^2-BN epilayers without a substrate that could influence the results.

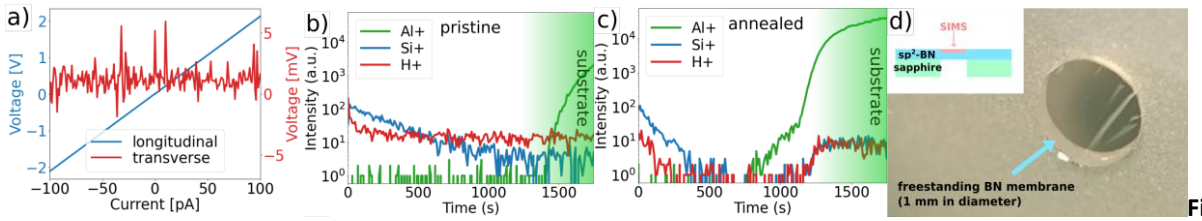


Figure 1. a) I-V measurements of a Hall bar fabricated from a conductive sp2-BN sample b) SIMS profile of the pristine c) and annealed sp2-BN layer on sapphire from the same growth process d) optical image and sheme of the freestanding membrane (layer thickness 38 nm).

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Acknowledgments

This research was supported in scope of NCN SONATA BIS 2024/54/E/ST7/00273

Friday 18.9.2026

Polymorphism and polytypism: from mineralogy to sp^2-bonded BN

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Controlling the stacking sequence of the 6-ring plane of alternating B and N atoms is an issue for the science of the sp2-bonded ultrawide bandgap semiconductor boron nitride. Its superior value of its fundamental bandgap compared to the bandgap of its challenger AlN permitts to target extremely short wavelengths of ligth emission either by second harmonic generation (SHG) [1] or using twisted pairs of thick BN layers[2,3]. SHG requires bulk crystalswithout lattice inversion symmetry, which is the case of the bernal (AB) stacking, the the rhombohedral stacking (ABC) and the AA stacking of BN layers[1,4,5,6]. Small individuals of such stacking can be obtained by heteroepitaxy [7] or by homoepitaxy of BN[7], large size epilayers are highly defective but can be obtained as dominantly made of AA' stacking[8,9] or twinned areas of rBN stacking embedded into AA' [10]. However, the isolation of large size bulk crystals is extremely difficult, even not possible, at the time being. I will discuss this issue in terms of the idea of epitaxy, syntaxy [11] and topotaxy[12,13,14]. The 2h-3r graphite case is also presented[15].

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Spin injection and emission helicity switching in a BA_2PbI_4/WSe_2 heterostructure

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The initialization of a long-lived spin population in lead halide perovskites is an essential prerequisite for their use in spintronic applications. We achieve this by using a $(BA)_2PbI_4/WSe_2$ monolayer heterostructure, shown schematically in Fig. 1(a). In this heterostructure, an interlayer exciton forms, due to the type II band alignment shown in Fig. 1(a). The photoluminescence (PL) spectrum is characterized by a broad peak at low energy, visible in Fig. 1(b,c), attributed to the interlayer exciton. The helicity resolved PL spectrum shows that the chiral optical selection rules of the WSe_2 monolayer influence the degree of polarization of the interlayer exciton, as shown in Fig. 1(b,c).

We performed polarization resolved PL excitation measurements across the exciton resonances shown in Fig. 1(d). Fig. 1(e) demonstrates that the circular dichroism of the interlayer exciton generally follows that of the WSe_2 intralayer exciton. The interlayer exciton displays a strikingly negative circular dichroism when the excitation laser is tuned in resonance with a heterostructure-related transition. The electronic coupling and charge transfer between WSe_2 and $(BA)_2PbI_4$ can be used to control the degree of circular polarization of the interlayer exciton [1].

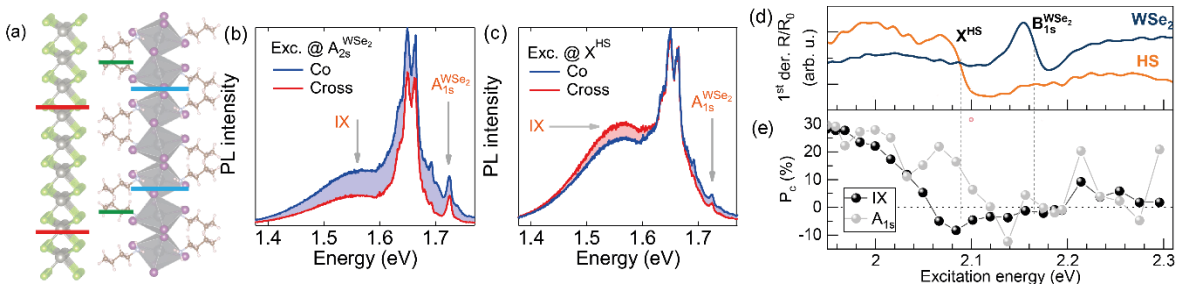


Figure 1. (a) Schematic of the $WSe_2/(BA)_2PbI_4$ heterostructure. The horizontal lines indicate the relative position of the band edges. Helicity-resolved PL spectrum of the WSe_2 monolayer/$(BA)_2PbI_4$ heterostructure for excitation in resonance with (b) the 2s exciton of WSe_2 (A_{WSe2}^{2s}) and (c) the X^{HS} transition. (d) First derivative of the reflectivity contrast spectrum measured on the WSe_2 monolayer and on the heterostructure. (e) Degree of circular polarization P_c of the interlayer exciton (opaque symbols) and of the 1s exciton of WSe_2 monolayer (transparent symbols) as a function of the excitation energy.

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Spectral shaping of SHG in hybrid hBN/rBN epitaxial stacks

J. Kossacki[1], B. Karim[2], F. Bojdecki[3], W. Zajkowska-Pietrzak[4], M. Bilska[1], J. Iwański[1], G. Szwed[1], I. Rogala[1], M. Pastorczak[2], A. K. Dąbrowska[1], J. Pawłowski[1], J. Binder[1], P. Wasylczyk[1], S. Kret[4], A. Wysmołek[1], T. J. Antosiewicz[1], and M. Klimczak[1]

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Hybrid epitaxial boron nitride combining the centrosymmetric hexagonal (hBN) and non-centrosymmetric rhombohedral (rBN) polytypes offer a unique platform for engineering second-order nonlinear optical response in the ultraviolet. We investigate how the spectral profile of second harmonic generation (SHG) in such heterostructures can be shaped by the combined action of stacking-induced optical interference and the intrinsic spectral dispersion of the rBN nonlinear susceptibility $\chi^{(2)}$. First-principles calculations of the wavelength-dependent $\chi^{(2)}$ of rBN are incorporated into transfer-matrix simulations of air/hBN/rBN/hBN/sapphire stacks, in which the top hBN cap and rBN thicknesses are varied at a fixed total thickness of 60 nm. The simulations reveal two distinct SHG regimes: in a localized-source regime of a relatively thin rBN with a thicker hBN cap, the excitation spectra are enhanced in the UV by about three-fold (Fig. 1a), whereas in an extended nonlinear-slab regime of a thick rBN with a thin or absent cap, this preference is lost (Fig. 1b). Control simulations assuming a dispersionless $\chi^{(2)}$ show that the observed non-monotonic spectral features require the interplay of stacking geometry and susceptibility dispersion and cannot be reproduced by geometry alone. SHG excitation spectra measured on polycrystalline MOVPE-grown BN films reproduce simulation results (Fig. 1c), identifying mixed-polytype epitaxial BN as a promising route toward compact UV nonlinear optical elements.

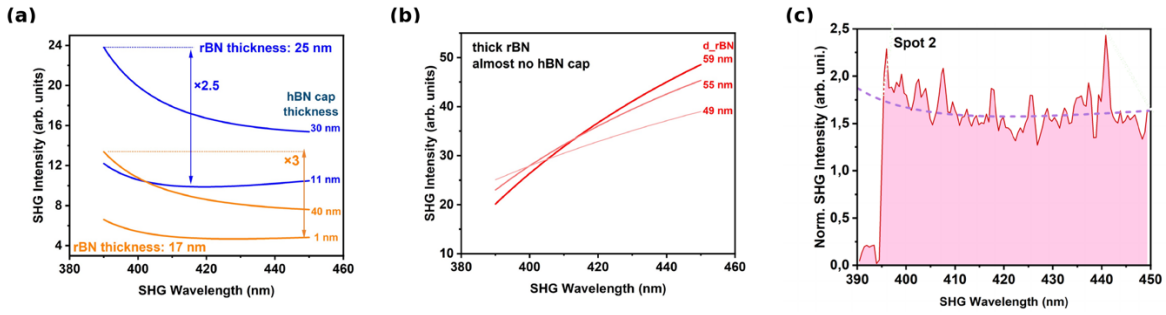


Figure 1. (a) Localized-source regime: simulated SHG excitation spectra are enhanced in the ultraviolet by a thick hBN cap; (b) Extended nonlinear-slab regime (almost no hBN cap): no SHG ultraviolet preference; (c) Measured SHG excitation spectrum (red) for a representative sample area with the corresponding transfer-matrix simulation (dashed violet).

Acknowledgments

Funded by the National Science Centre, Poland, grant OPUS 2023/51/B/ST7/01204. Computations were partially performed at ICM, University of Warsaw (grant GC84-51).

Periodic Excitation of Magnons in CrSBr

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Magnons play a significant role in quantum technology, material science and solid-state physics. Their small wavelengths make them compatible with quantum nano-devices, and their frequencies can surpass modern computation speeds. This potential makes them useful for various elements in quantum computing networks. In this work we present a novel experimental method based on the all-optical periodic pump-probe excitation and detection of magnons. Here we investigate 2D materials that combine long-range magnetic order with semiconducting character- CrSBr and CrS(Br,I).

This study focuses on resonant excitation of coherent magnons in time domain by generating a train of pump pulses in Fabry-Perot resonator that match the resonant frequency of the modulated collective excitation. By doing so one can enhance the amplitude of coherent response of the system and narrow down the spectral line of such excitation depending on the system parameters. By changing the repetition rate of pumping it is possible to filter out and address magnon mode with a particular frequency enabling selective excitation of particular layers in the stack of 2D materials.

Presented results are based on previous studies on periodic pumping of magnons in GeFe [1]. Current experiments are aimed to establish optimal parameters of excitation such as time profile and power, depending on the system.

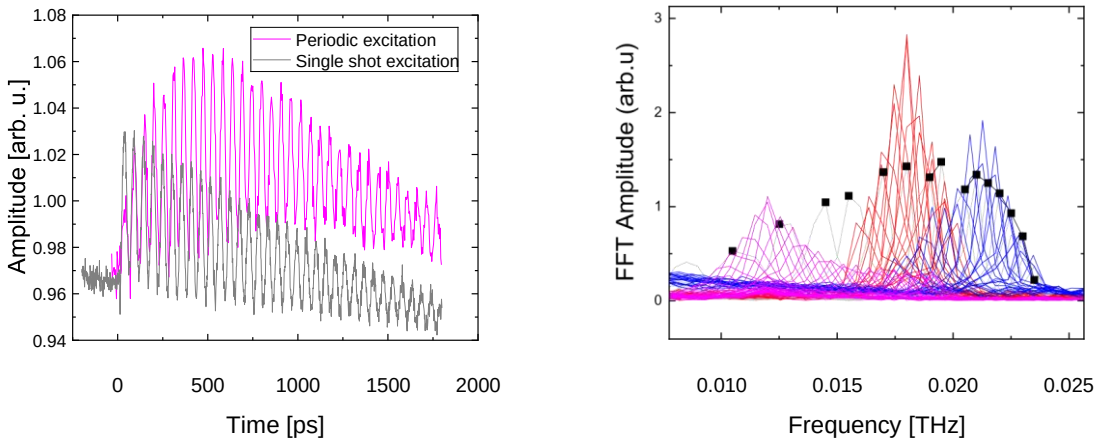


Figure 1 a) time trace of magnetization precession in CrSBrI, single shot excitation compared to periodic excitation by subsequent train of pulses. b) FFT amplitudes of signals for single shot excitation (gray+dots) compared to periodic excitation for various repetition rates (color plots) in the function of magnetization precession frequency tuned by external magnetic field.

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$MoTe_2$ for infrared photonics

Marcin Syperek

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$MoTe_2$ in its 2H allotropic form (2H-$MoTe_2$) is a particularly attractive transition-metal dichalcogenide for near-infrared photonics, with fundamental excitonic transitions at wavelengths above 1 μm. In this talk, I will focus primarily on the electrical control of the optical response of monolayer (ML) $MoTe_2$ and on using electrostatic doping as a quantitative tool to extract device-independent material parameters [1]. I will also discuss Coulomb engineering via dielectric screening [2] and strong light–matter coupling in ML and bilayer (BL) $MoTe_2$ [3].

In gated ML $MoTe_2$, photoluminescence and contrast-reflectivity spectroscopy reveal systematic changes of neutral- and charged-exciton energies and oscillator strengths with carrier density. Calibration of the carrier concentration from the device capacitance allows the optical response to be expressed directly as a function of electron or hole density. This provides access to charge-dependent energy shifts, the Fermi energy, exciton–trion separation, and saturation densities. Analysis of phase-space filling yields an exciton Bohr radius of approximately 0.7–0.8 nm, while the trion-to-exciton oscillator-strength ratio gives a trion radius of about 2.4–2.8 nm.

A complementary tuning mechanism is dielectric screening of the Coulomb interaction. By placing ML and BL $MoTe_2$ in different dielectric environments, the quasiparticle gap and exciton and trion binding energies can be modified, resulting in optical-transition shifts of up to approximately 19 meV in the monolayer and 8 meV in the bilayer.

Finally, I will discuss cavity electrodynamics in $MoTe_2$. Coupling excitonic resonances to confined modes of a tunable open microcavity produces clear exciton-polariton anticrossing, with Rabi splittings of about 13 meV for ML and 18 meV for BL $MoTe_2$. The monolayer exhibits a polariton-relaxation bottleneck, whereas the bilayer shows efficient relaxation into the lower polariton branch.

Together, electrostatic doping, dielectric screening, and cavity coupling provide complementary routes for controlling the electronic, excitonic, and photonic properties of $MoTe_2$ for active infrared and quantum photonics.

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Magneto-Optics of Bright and Dark Excitons in a $MoWSe_2$ Monolayer Alloy

M. R. Molas

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Monolayers (MLs) of semiconducting transition-metal dichalcogenides (S-TMDs), such as $MoSe_2$ and WSe_2, have direct band gaps and strong excitonic effects that govern their optical emission and absorption [1]. Depending on the spin configuration of the lowest excitonic state, they can be classified as bright, as in $MoSe_2$, or darkish, as in WSe_2, while $Mo_xW_{1-x}Se_2$ alloys enable continuous tuning of the emission energy through the Mo/W composition.

The first part of my talk will be devoted to the investigation of the magneto-optical properties of excitonic complexes in $Mo_xW_{1-x}Se_2$ MLs encapsulated in hexagonal BN (hBN) with different Mo/W ratios [2]. Under applied magnetic fields, the neutral exciton resonances in S-TMD MLs split into two circularly polarized components as a result of the Zeeman effect [2]. Using low-temperature photoluminescence (PL) experiments performed in external outof-plane magnetic fields up to 30 T, we extract the g-factors of the neutral (X) and charged (T) excitons. The g-factors of the X transitions vary gradually from approximately −4 to approximately −10. This striking tunability is supported by first-principles band-structure calculations, which reproduce the experimental trend.

In the second part, I will present our investigation of the low-temperature PL of an hBN-encapsulated $Mo_{0.68}W_{0.32}Se_2$ ML under in-plane magnetic fields, ($B_{\parallel}$), up to 25 T [3]. At zero field, the PL spectrum resembles that of a bright $MoSe_2$ ML, with two well-resolved lines, X^B and T, assigned to the neutral and charged bright excitonic complexes, respectively. Above $B_{\parallel} \sim 15$ T, an additional emission line, X^D, emerges 14.2 meV below X^B. Its intensity follows a quadratic field dependence, $I^{XD} \sim \alpha B_{|}^2|$, confirming its assignment to the magnetic-fieldbrightened dark excitonic ground state. We also observe a strong quenching of the X^B emission with increasing $B_{\parallel}$, which we describe using a model of in-plane-field-induced bright-dark exciton coupling. By diagonalizing a coupled 2×2 Hamiltonian and fitting the field evolution of the X^B and X^D energies, we obtain an in-plane excitonic g-factor of g=5.2±0.2. Assuming thermal equilibrium, the model predicts a 92% reduction in the bright-exciton population, in good agreement with the experimentally observed 85% decrease.

Together, these results demonstrate that alloy composition and magnetic-field orientation provide complementary means to tune and probe the exciton landscape in $Mo_xW_{1-x}Se_2$ MLs.

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[3] K. Olkowska-Pucko *et al.*, under preparation.

Extremely High Excitonic *g*-Factors in 2D Crystals by Alloy-Induced Admixing of Band States

Tomasz Woźniak,[1] Katarzyna Olkowska-Pucko,[2] Elena Blundo,[3] Paulo E. Faria Junior[4], Adam Babiński[2], Antonio Polimeni[5] and Maciej Molas[2]

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Monolayers of semiconducting transition metal dichalcogenides (TMDCs) emit light very efficiently and display rich spin-valley physics, with excitonic *g*-factors of about −4. Vertical heterostructures based on TMDCs can host excitonic complexes with much larger *g*-factors, that can be tuned by interlayer twist angle and stacking registry. These parameters are, however, not easy to control during preparation of the samples. Because of the much simpler fabrication process of monolayers compared to heterostructures with specific twist angles, alloying of TMDCs opens new avenues for valleytronic and quantum devices. Recently, we have shown by magnetooptical spectroscopy and theoretical calculations that mixed (Mo,W)Se_2 monolayers at certain compositions exhibit significantly larger exciton *g*-factors than the parent crystals [1]. Density functional theory-based summation-over-bands calculations [2] revealed a strongly non-linear *g*-factor dependence on the alloy composition. We explain it in terms of resonant hybridization of K and Q valley states in the conduction band. Moreover, the compositional dependence of *g*-factors can be additionally tuned by applying mechanical strain.

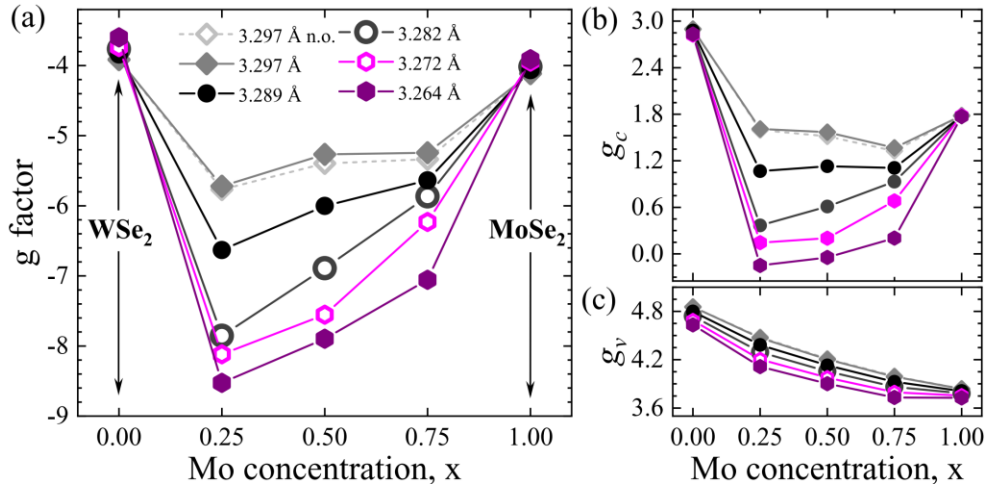


Figure 1. Calculated compositional dependence of *g*-factors of (a) excitons, (b) conduction and (c) valence bands at K points for different lattice constants.

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Poster presentations

(alphabetical order)

Wednesday

16.9.2026

Integrated Photonic Platform for Electrical Control of Nanoscale Light Emission

Patrycja Dembek[1], Paweł Holewa[1,2], Christian Ruiz[2], Katarzyna Gwóźdź[1], Zdeněk Sofer[3], Elizaveta Semenova[2], Marcin Syperek[1]

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The control of light emission from van der Waals (vdW) materials requires device architectures that allow the optical response of a transferred flake to be modified by its local environment. In particular, local strain can create spatially confined emission sites, while electrostatic gating can tune the charge state, emission energy, and stability of optical transitions. In this presentation, we demonstrate an integrated photonic platform designed to combine these two control mechanisms within a single electrically addressable structure. The platform consists of an Au bottom gate/back reflector, an Al_2O_3 dielectric spacer, lithographically defined top electrodes, and HSQ nanopillar arrays used to locally deform transferred vdW flakes, as schematically shown in Fig. 1. Such a structure enables the active material to be incorporated into a capacitor-like gate geometry while maintaining optical access to strain-engineered emission sites.

The fabricated platform was characterized structurally, electrically, and optically. These measurements confirmed the successful realization of the designed multilayer architecture, verified electrical access to the gate structure, and helped define the practical operating range of the device. These results validate the structure as a basis for future experiments combining local strain, electrostatic gating, and optical-field engineering in vdW light emitters.

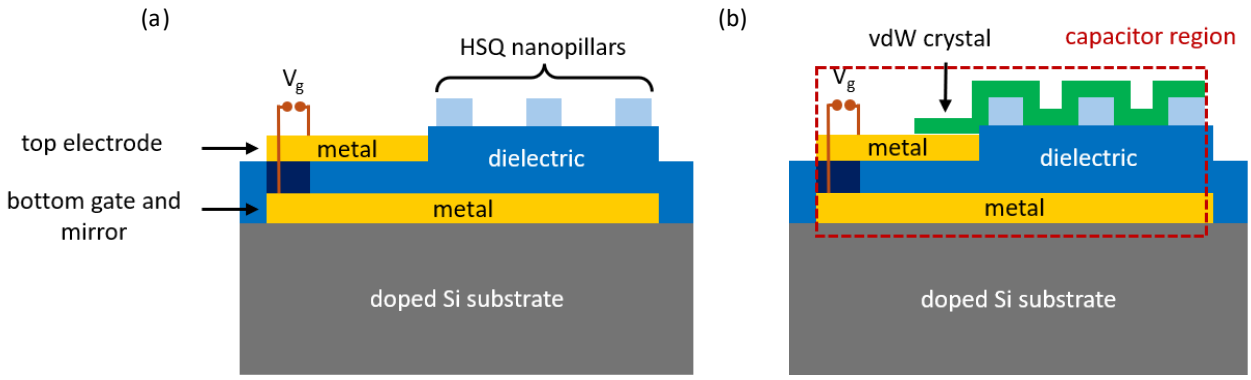


Figure 1. Schematic cross-section of the integrated photonic platform: (a) fabricated electrode/dielectric/nanopillar architecture, (b) vdW flake integrated with the active capacitor region for combined strain and electrostatic control of light emission.

The Impact of Annealing on the Photoluminescence of Negatively Charged Boron Vacancies in Epitaxial Boron Nitride

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Layered sp^2-bonded boron nitride (sp^2-BN), also referred to as layered BN, is a wide-bandgap two-dimensional (2D) material and a promising candidate for use in van der Waals heterostructures and as a host for optically addressable spin defects. One such defect is the negatively charged boron vacancy (V_B^-), an isolated optically active spin center that can be created via slow neutron irradiation, with broad potential applications in quantum sensing technologies. The emergence of these spin defects is observed as a broad emission band in the photoluminescence (PL) spectrum of sp^2-BN in the near-infrared (NIR) range (Fig. 1) [1]. The significant spectral broadening results from strong electron–phonon coupling and phonon-assisted recombination, phenomena commonly observed in solid-state systems [2].

Post-irradiation annealing may initiate a range of crystal structural modifications, such as migration and defect clustering, which may lead to a reduced concentration of isolated boron vacancies and give rise to non-radiative recombination pathways.

We investigate the temperature-dependent PL spectrum evolution of several annealed and non-annealed layers of epitaxial sp^2-BN grown on a 2-inch sapphire substrate. The observed changes constitute a significant advance in the understanding of the creation and evolution mechanisms of V_B^- in layered BN and are essential for controlled defect engineering crucial for future applications.

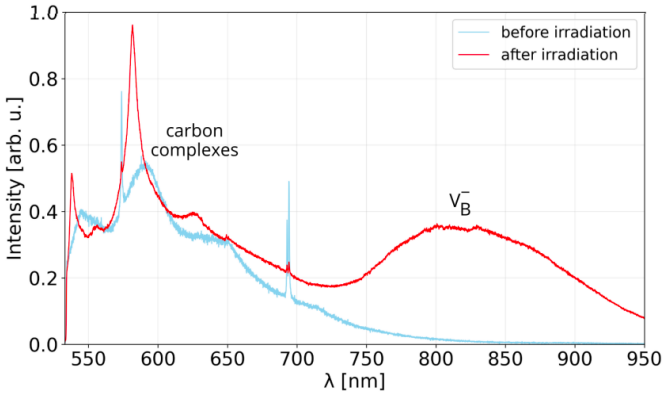


Figure 1. Photoluminescence spectrum of epitaxial sp^2-BN before and after irradiation.

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Acknowledgments

This work was partially supported by the National Science Centre of Poland, grant no 2022/47/B/ST5/03314.

Photoluminescence of $MoSe_2$ doped with rhenium (Re) and niobium (Nb)

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Atomically thin films of transition metal dichalcogenides (TMDs) are a versatile class of two-dimensional semiconductors. Due to their remarkable optical and electronic properties, they represent a promising group of materials for optoelectronic applications. Among them, $MoSe_2$ has attracted scientific interest because of its strong excitonic response and tunable band structure [1]. Doping of these compounds is an effective method for modifying the electronic structure and carrier concentration, thus altering optical properties and possibe applications.

In this work, $MoSe_2$ crystals doped with rhenium (Re) and niobium (Nb) were investigated. Rhenium and niobium are expected to be a donor (n-type) dopant and aceptor (p-type) dopant, respectively [2]. We present the results of photoluminescence (PL) studies of monolayers as a function of temperature (5-300 K) and dopant content (0%, 0.1%, 1%, 3%). The addition of Re to $MoSe_2$ significantly attenuates the photoluminescence of the monolayer, and the higher the Re content, the greater the attenuation. However, the addition of Nb in a smaller amount (up to 1%) increases the luminescence, but further increasing its content causes the photoluminescence decreases. Moreover, the peak position shifts to lower energies at higher Nb content.

The comparative analysis allows for a better understanding of the influence of donor (Re) and acceptor (Nb) doping on the recombination mechanisms and optical response of monolayer $MoSe_2$. Some dopants concentration result in PL enhencement. This phenomena can play the role in the design of advanced optoelectronic devices.

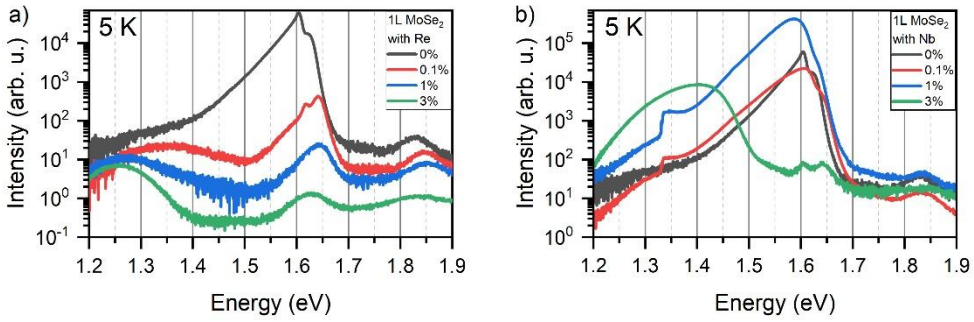


Figure 1. Photoluminescence spectra obtained for the monolayers of $MoSe_2$ undoped and doped with (a) rhenium, (b) niobium at 5 K as a function of the admixture content.

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Spectroscopic Investigation of Interlayer Excitons in hBN/WS_2/WSSe van der Waals Heterostructures

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Transition metal dichalcogenides (TMDCs, MX_2), such as WS_2, MoS_2, $MoSe_2$, and WSe_2, are layered two-dimensional materials with an X–M–X atomic structure. Recent advances in alloy synthesis have enabled compositions $WS_{2(1-x)}Se_{2x}$; in this work, $WS_{0.5}Se_{1.5}$ and $WS_{0.5}Se_{0.5}$ were investigated. Their strong in-plane covalent bonding and weak interlayer van der Waals interactions allow mechanical exfoliation into monolayers, which exhibit a direct band gap and strong photoluminescence. Optical excitation followed by charge transfer between adjacent layers forms interlayer excitons with long lifetimes (1–100 ns), high binding energies (about 100 meV), and twist-angle-dependent properties.

Van der Waals heterostructures were fabricated by deterministic all-dry stacking of mechanically exfoliated TMDCs and hBN on Si substrates. Two interlayer excitons (IX_1 and IX_2) were identified at 1.52 and 1.60 eV (7 K). Temperature-, power-, and Raman-dependent measurements were performed to characterize the structures. In addition, polarization-resolved photoluminescence excitation (PLE) and upconversion photoluminescence (UPC) measurements were carried out to investigate the excitation-energy dependence, polarization properties, and the nature of the interlayer exciton states. These measurements were used to determine which interlayer exciton corresponds to the ground state and which originates from the moiré potential. The comprehensive optical characterization provides further insight into interlayer excitons in mechanically exfoliated TMDC heterostructures.

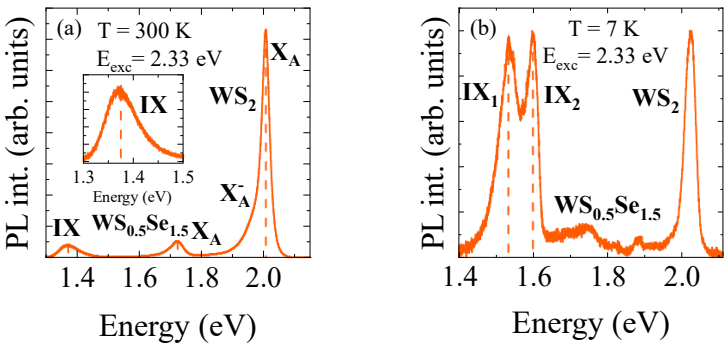


Figure 1. (a) PL spectrum measured at room temperature under an excitation energy of $E_{\mathrm{exc}} = 2.33$ eV. (b) PL spectrum measured at $T = 7$ K under an excitation energy of $E_{\mathrm{exc}} = 2.33$ eV.

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Exciton and magnon dynamics in CrSBr studied with excitation correlation spectroscopy

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CrSBr is a two-dimensional (2D) van der Waals magnetic material exhibiting an A-type antiferromagnetic order below the Néel temperature (T_N = 132 K) [1]. It is of great interest due to its exceptionally strong coupling between optical and magnetic properties. The optical response in PL shows distinct excitonic states in the energy range of 1300-1400 meV. The direct coupling of excitons with the magnetic order provides optical access to magnons, making this system an ideal platform for understanding its dynamics.

In this work, we present the study of exciton relaxation dynamics and their dependence on the magnetic alignment in a quasi-bulk CrSBr flake. We combine different experimental techniques, including time-resolved photoluminescence (TRPL) and excitation correlation spectroscopy (ECS). The results obtained with the latter technique were particularly interesting. Under excitation by two delayed pulse trains (fs Ti:Sapp laser), we measured the time-integrated PL spectra. The delay between the laser pulses was scanned in order to probe the interaction between both excitations with sub-picosecond resolution.

We performed measurements from zero magnetic field up to the saturation field, at which the material turns into the ferromagnetic orientation. At zero magnetic field, temporally overlapping pulses reveal Auger recombination as the main nonlinear PL quenching mechanism. Furthermore, an external magnetic field accelerates exciton dynamics, shortening their lifetime. Interestingly, distinct magnon oscillations emerge in the PL signal at intermediate magnetic field values. The observed magnon frequency dispersion matches results delivered from pump-probe technique, but ECS achieves this with a significantly simpler setup, eliminating the need to tune the probe pulse to the exciton energy, enabling investigation of magnon dynamics for everyone equipped in pulsed laser [2].

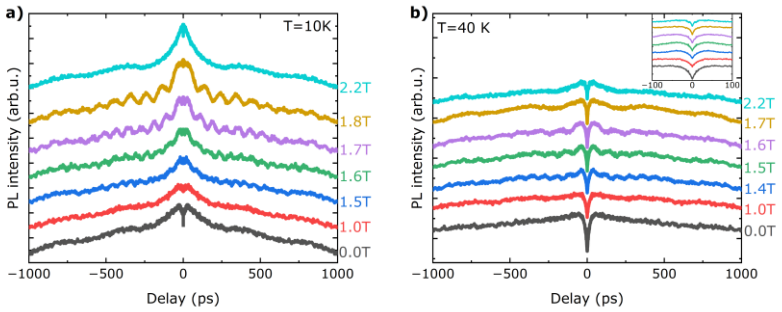


Figure 1. Time-integrated PL intensity as a function of delay between laser pulses. a) For 10 K. b) For 40 K.

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Study of the operating temperature of two-dimensional transistors via Raman spectroscopy

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Two-dimensional semiconductors, such as transition metal dichalcogenides, are considered promising materials for future electronic devices due to their atomically thin structure and the resulting potential for improved electrostatic control at reduced device dimensions [1]. However, continued device miniaturization is accompanied by increasing challenges related to heat generation and dissipation. Joule heating can lead to a significant local temperature rise in the active channel, affecting carrier transport, device performance, and long-term reliability [2]. Understanding how heat is generated and transferred from the active layer to the surrounding structure is therefore essential for the development of reliable electronic devices based on two-dimensional materials.

In this work, Raman thermometry is used to investigate self-heating and heat dissipation in field-effect transistors based on monolayer MoS_2. The temperature response of both the MoS_2 channel and the silicon substrate is analyzed during electrical operation, enabling insight into heat transfer from the active layer to the underlying structure. The study examines the influence of the dielectric material and channel geometry on the electrothermal behavior of the devices, as well as the spatial temperature distribution along the transistor channel. Additionally, devices incorporating a metallic layer beneath the dielectric are investigated to assess how modifications of the device architecture affect heat dissipation and thermal stability.

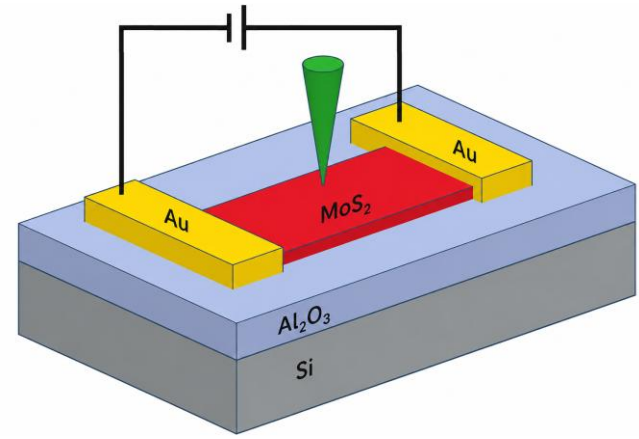


Figure 1. Schematic illustration of the investigated monolayer MoS_2 field-effect transistor on an Al_2O_3/Si substrate during Raman thermometry measurements.

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Synthesis of Borophene-like nanosheets via Chemical Vapor Deposition on Copper Substrate

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Borophene, a recent addition to the two-dimensional material family, has aroused significant interest due to its unique crystal structures, metallic character, and extraordinary physical properties. In comparison with other two-dimensional materials, borophene exhibits a unique combination of high electrical conductivity, mechanical flexibility, and an isotropic structure, making it a promising candidate for next-generation functional materials in catalysis and nanoelectronics [1]. Despite these attractive properties, the scalable preparation and controlled growth of high-quality borophene sheets remain challenging.

Among the alternative approaches, bottom-up synthesis strategies have emerged as attractive routes due to their potential for large-scale production. In such processes, the choice of substrate and carrier gas plays a crucial role, as it directly affects the precursor decomposition, surface nucleation, and crystal quality. Since the experimental environment is one of the key factors governing the efficiency and stability of two-dimensional boron growth, understanding the influence of reaction parameters is crucial for optimizing the production of boron-based nanosheets [2].

In this work, Chemical Vapor Deposition (CVD) was investigated as a path for the preparation of few-layer borophene-like nanostructures on a copper substrate. The process was carried out in a hydrogen environment, evaluating the influence of different reaction times, including 15 min, 30 min, 1 h, and 2 h. The prepared materials were examined using methods like X-ray Diffraction (XRD), X-ray Photoelectron Spectroscopy (XPS), Atomic Force Microscopy (AFM), and Transmission Electron Microscopy (TEM).

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Acknowledgments

This research has received funding from the National Science Centre (Poland) with grant OPUS21 number (2021/41/B/ST5/03279).

Temperature-dependent Raman response of mixed $Fe_xMn_{1-x}PS_3$ layered antiferromagnets

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Layered transition metal trichalcogenophospites MPX_3 are quasi-two-dimensional antiferromagnetic semiconductors that have attracted considerable attention owing to their tunable magnetic anisotropy, sizable band gaps, and strong spin–lattice coupling. Among them, $FePS_3$ and $MnPS_3$ represent two limiting cases with distinct Néel temperatures and magnetic symmetry, and they exhibit characteristic Raman fingerprints of magnetically driven phonon renormalization and magnon-related excitations [1, 2, 3].

In this work, we investigate bulk and exfoliated mixed $Fe_xMn_{1-x}PS_3$ crystals by temperature-dependent Raman spectroscopy, focusing on the evolution of selected phonon modes in the low-temperature regime as a function of the Fe/Mn ratio.

The Raman spectra reveal systematic, composition-dependent shifts and linewidth changes of several modes, as well as an intensity redistribution that becomes particularly pronounced in the vicinity of the magnetic transitions characteristic of the $FePS_3$– and $MnPS_3$–rich compositions. For intermediate compositions, we observe pronounced anomalies of modes in the 100–180 cm^{-1} range, which deviate from purely anharmonic temperature trends and indicate enhanced spin–phonon coupling and magnetoelastic interactions, similar to those reported for pure $MnPS_3$ and $FePS_3$ but modified by cation substitution. These results demonstrate that chemical mixing in $Fe_xMn_{1-x}PS_3$ provides an effective route to engineer the interplay between lattice vibrations and magnetic correlations in van der Waals antiferromagnets, and they highlight Raman spectroscopy as a sensitive probe of spin–lattice coupling in tunable two-dimensional magnetic materials.

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2D Selenides for electro-optical research

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Two-dimentsional nanomaterials (2D nanomaterials) are composed of thin layers that may have a thickness of at least one atomic layer. These atoms have a different function than internal atoms, and so the increase in the number of surface atoms leads to a change in the behavior of 2D nanomaterials [1]. As a result of which contrary to bulk materials, these nanomaterials have unique features of high aspect ratio (surface-area-to-volume ratio), anisotropy, electron confinement, and optical properties. They are extensively explored for membranes, energy production/storage, tissue engineering, sensing, and catalytic applications.

Two-dimensional (2D) selenides has attracted intensive attention as a promising material candidate for future optoelectronic applications. Successfully synthesized in 2017, 2D molybdenum selenide exhibits advanced properties, including size-dependent bandgap, strong photoluminescence effect, anisotropic thermal conductivity, and high photoconductivity, render it and selenium-based composites a promising candidate for various device applications [2].

In this work, sonochemical exfoliation was investigated as the foundation for obtaining two-dimensional (2D) Molybdenium and Tin selenides, respectively. The process was carried out in ultra clean water by means of ultrasound horn for 4 hours, and then the material was dried on a hot plate until the solvent evaporated. The prepared materials were examined using methods such as atomic force microscopy (AFM), X-ray Diffraction (XRD), Transmission Electron Miscroscopy (TEM) and a series of electrocatalytic experiments.

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Influence of pulsed and continuous wave laser excitation on energy transfer in type-II heterostructures

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Type-II heterostructures (HSs) of transition metal dichalcogenides (TMDs) show F¨orstertype resonant energy transfer (ET) mediated by dipole-dipole interactions between the excitons present in the donor layer and the acceptor layer [1]. Such ET processes were typically investigated under either continuous-wave (cw) or pulsed excitation. The influence of the excitation temporal profile on excitonic population and interlayer coupling remains unexplored. In this work, we systematically compare ET in a WS_2/hBN/MoS_2 HS (Fig. a), where energy transfer occurs from MoS_2 to WS_2, under conditions that are identical in all parameters except for the nature of the excitation (cw versus pulsed).

The photoluminescence (PL) intensity of the HS is significantly higher under cw excitation than under pulsed excitation, as shown in (Fig. b). This indicates that cw excitation maintains a steady exciton population which enables continuous and efficient ET. In contrast, pulsed excitation generates a large number of excitons within a short temporal window, which promotes non-linear processes and reduces the ET efficiency. In further experiments, power dependent measurements have been performed using cw and pulsed excitations, shown in (Fig. c), which reveal that at high pulsed excitation powers, the integrated intensity of the WS_2 exciton in the HS deviates from linear behavior and shows saturation, whereas under cw excitation behavior remains linear, as for measurements on isolated WS_2 regardless of the nature of the excitation. These findings highlight the importance of non-equilibrium exciton dynamics in optoelectronic science and suggest that direct comparisons between cw and pulsed excitation provide valuable insight into carrier interactions and nonlinear processes in van der Waals HSs.

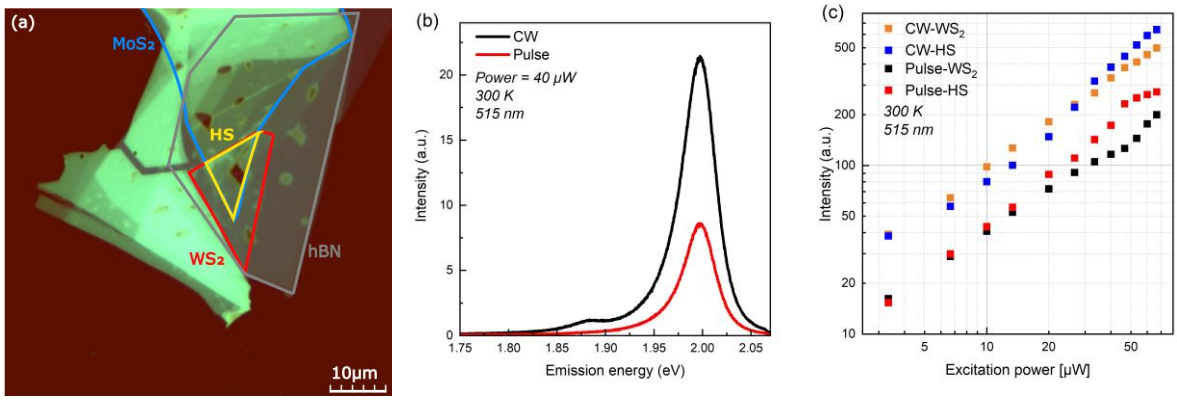


Figure 1: (a) Optical image of the hBN/MoS_2/hBN/WS_2/hBN/SiO_2. (b) Photoluminescence (PL) spectra of HS under cw and pulsed excitation. The PL emission under CW is significantly higher than under pulsed excitation at the same power. (c) Integrated PL intensity of the WS_2 exciton in HS and in isolated WS_2 as a function of excitation power (log-log scale). A deviation from linear scaling of the HS is visible under high pulsed excitation power. This indicates saturation. Response remains linear for isolated WS_2 and for HS under CW.

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Electrolyte Additive Engineering for Interfacial Stability of Al Anodes in Aqueous Aluminum Metal Batteries: Sodium Molybdate and Glutamic Acid

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Aqueous aluminum metal batteries hold great promise for grid-scale energy storage due to their low cost and high safety. However, the Al anode suffers from severe Cl^--induced pitting corrosion and hydrogen evolution in $AlCl_3$ aqueous electrolytes, critically limiting the cycle life. This work systematically investigates two types of additives—inorganic sodium molybdate (Na_2MoO_4) and natural amino acid glutamic acid—for their regulatory mechanisms on Al anode corrosion behavior.

In the molybdate system, 10 mM Na_2MoO_4 enables the Al||PBA full cell to achieve a capacity retention of 67.4% after 400 cycles at 250 mA g^{-1}. XPS and TOF-SIMS analyses reveal that MoO_4^{2-} preferentially adsorbs onto the Al_2O_3 surface, competitively interacting with Cl^-, and undergoes in-situ electrochemical reduction to form a protective MoO_2/MoO_3 deposition layer with Cl^- embedded within, thereby transforming the corrosion mode from localized pitting to uniform dissolution.

In the amino acid system, 20 natural amino acids were systematically screened, and glutamic acid was identified as the most effective corrosion inhibitor at 0.3 M. Under identical testing conditions (250 mA g^{-1}, 0.5–1.7 V), the Al||PBA full cell achieves a capacity retention of 81.5% after 400 cycles. The inhibition mechanism is attributed to the synergistic adsorption of its three functional groups (two carboxyl groups and one amino group) on the Al surface, which effectively repels Cl^- attack and guides a uniform Al^{3+} flux.

This work provides a dual-strategy reference for electrolyte additive design in low-cost, long-lifetime aqueous aluminum metal batteries, ranging from inorganic protective deposition layers to organic functional group synergistic adsorption.

Terahertz Spectroscopic Insights into Nanomaterials Derived from Liquid Phase Exfoliation

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In this study, a range of nanomaterials produced via liquid phase exfoliation (LPE) were investigated alongside reference layered and bulk materials. The aim was to examine how differences in internal structure, origin, and fabrication route influence the terahertz (THz) optical and electronic properties of these systems. Terahertz time-domain spectroscopy (THz-TDS) was employed to determine key optical parameters, including the refractive index (n), absorption coefficient (α), and frequency-dependent conductivity (σ'). Significant variations in the THz response were observed among the studied materials, reflecting differences in flake morphology, layer stacking, defect density, and charge transport mechanisms. The terahertz-range conductivity was analyzed, providing insight into carrier localization and backscattering effects characteristic of disordered and nanostructured systems. To establish structure-property relationships, complementary characterization techniques such as Raman spectroscopy, X-ray diffraction, UV-Vis spectroscopy and scanning electron microscopy (SEM) were performed, enabling a comprehensive correlation between microstructural features and the observed optical and electronic behavior.

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Influence of the Environment on MoS_2 Thermal Conductivity Measurements

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Thermal conductivity (κ) plays a crucial role in the development of nanoscale electronics and thermal management devices [1]. However, the wide variation in measurement techniques frequently leads to fundamentally divergent results across studies. These discrepancies may stem from environmental influences during data acquisition, such as the presence of ambient air versus a vacuum.

In the present work, we aimed to investigate how environmental conditions impact the κ measurements of suspended MoS_2. Utilizing Raman thermometry, we systematically compared data acquired under vacuum and in ambient air [2]. However, we found that immediate data acquisition following chamber evacuation or venting is precluded by transient shifts in the Raman shift positions, necessitating an extended stabilization period. To precisely isolate the effect of the gaseous environment, we designed specialized architectures that facilitated the extraction of air trapped beneath the MoS_2 layer (Figure 1). Interestingly, the apparent κ values measured in air are significantly higher than those obtained in a vacuum, primarily due to convective heat dissipation into the surrounding atmosphere. Consequently, the power-dependent Raman shifts (specifically the red-shifts of the A and E modes) exhibit noticeably steeper, more negative slopes under vacuum conditions. This trend persists in multi-layer MoS_2, but added layers introduce competing effects that reduce the environmental impact.

The poster will highlight these key discrepancies and provide detailed insights into the mechanisms driving environmental influence in MoS_2 thermal conductivity measurements.

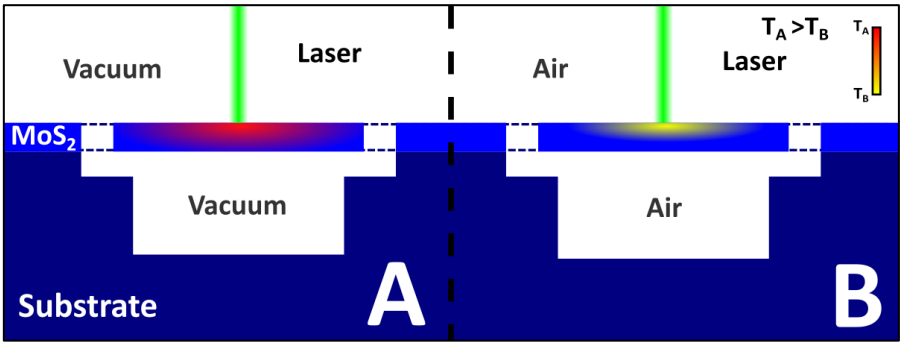


Figure 1. Schematic comparison of samples in vacuum (A) and air (B). The MoS_2 layer experiences more intense heating in a vacuum.

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Acknowledgments

The authors acknowledge financial support from the Polish National Science Centre under the OPUS grant No. 2025/57/B/ST11/02260.

Correlated Electrical Transport and Exciton–Phonon Coupling in Monolayer $MoWSe_2$ Driven by Environmental Adsorbate Desorption

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Ternary transition-metal dichalcogenide (TMD) alloys offer a versatile platform for tuning the electronic and optical properties of two-dimensional semiconductors through compositional control. However, the relationship between environmental adsorbates, interfacial electrostatics, charge transport, and excitonic properties in ternary TMDs remains poorly understood. Here, we investigate the effect of adsorbate desorption on monolayer $Mo_{0.5}W_{0.5}Se_2$ using FM-KPFM, back-gated field-effect transistors with Au and Pd contacts, and temperature-dependent Raman and photoluminescence spectroscopy in nitrogen and vacuum environments. Combining local electrostatic measurements with electrical and optical characterization reveals a common influence of surface adsorbates on carrier injection, transport, and exciton–phonon interactions. Upon adsorbate desorption, the carrier mobility increases by nearly four orders of magnitude, while the on-state current increases by approximately two orders of magnitude, indicating substantially improved carrier transport and metal–semiconductor injection. At the same time, changes in the temperature-dependent photoluminescence and exciton linewidth demonstrate modified exciton–phonon interactions. These results establish a direct link between interfacial electrostatics, charge transport, and optical response, highlighting environmental adsorbates as a key factor governing the properties of monolayer $Mo_{0.5}W_{0.5}Se_2$.

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Subwavelength gratings based on epitaxial $MoSe_2$

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Transition metal dichalcogenides (TMDs), including molybdenum diselenide ($MoSe_2$), are a promising platform for nanophotonics, due to their strong excitonic resonances, nonlinear properties, and – last but not least – extremely high refractive index (~4.4 in the near infrared). In this paper, we demonstrate the design and realization of bound states in the continuum (BICs) in subwavelength gratings fabricated from epitaxially grown $MoSe_2$.

We grew high-quality, large-area $MoSe_2$ layers by using Molecular Beam Epitaxy (MBE). The layers are patterned into subwavelength gratings hosting symmetry-protected BICs in the near infrared. This strong light-matter interaction in the BICs leads to a giant enhancement of third-harmonic generation (THG) by more than three orders of magnitude compared to an unpatterned epitaxial $MoSe_2$ layer. Our results show the potential of epitaxial TMDs as materials for flat, non-linear optoelectronic and photonic devices.

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Influence of Substrate Type on the Growth of Molybdenum Oxide Structures Deposited by Physical Vapor Deposition

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Molybdenum oxide thin films were deposited by physical vapor deposition (PVD) onto three different substrates: freshly cleaved mica, gold-coated mica (Au/mica), and silicon wafers covered with a 270 nm silicon dioxide (SiO_2) layer. The influence of substrate type on the morphology and growth behavior of the deposited molybdenum oxide structures was investigated. Surface characterization revealed notable differences in the distribution, size, and arrangement of grown objects depending on the substrate properties. Mica provided a smooth crystalline surface that promoted uniform object formation, while the conductive Au/mica substrate affected nucleation and growth processes, resulting in distinct surface features. On Si/SiO_2 substrates, the amorphous oxide layer influenced the morphology and spatial distribution of the deposited objects. These observations demonstrate that substrate composition and surface characteristics play a significant role in determining the structural properties of PVD-grown molybdenum oxide.

Acknowledgments

This work was financially supported by the University of Lodz under the National Science Centre, Poland, under the Grant NCN 2024/55/B/ST11/01717

Comparative study of Sb_2O_3 on HOPG and mica

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Antimony(III) oxide (Sb_2O_3) has recently emerged as a promising dielectric material for next-generation two-dimensional (2D) electronic devices owing to its wide band gap, favorable dielectric properties, and molecular crystal structure based on van der Waals interactions. These characteristics enable the formation of high-quality interfaces with layered materials, making Sb_2O_3 an attractive candidate for 2D heterostructures.

In this work, the growth of Sb_2O_3 on layered substrates, namely mica and highly oriented pyrolytic graphite (HOPG), was investigated. The material was synthesized using two deposition approaches: growth under atmospheric conditions and under ultra-high vacuum (UHV). The obtained structures were characterized by atomic force microscopy (AFM) and Raman spectroscopy. The results reveal distinct morphological and structural features depending on the growth conditions and confirm the successful formation of Sb_2O_3 layers on both substrates.

These findings contribute to the understanding of Sb_2O_3 growth mechanisms and support its potential application as a dielectric component in future 2D electronic systems.

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This work is supported by the National Science Centre, Poland, under the Grant NCN 2024/55/B/ST11/01717.

Characterization of graphene nanoplatelets using THz-TDS

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A graphene flake consists of several to a dozen or so layers of graphene and has specific surface area ranging from several hundred nanometers to micrometers [1]. The aim of this research is to determine the physical properties of commercially available graphene flakes using terahertz time-domain spectroscopy (THz-TDS). The key components of the setup are: a femtosecond laser, a delay line, and a THz transmitter and receiver [2]. Measurements in the terahertz range were performed on pellets with a polyethylene matrix and graphene flakes as the active material at mass concentrations of 1% or 0.4%. To this end, 10 samples of various graphene flakes were used, and their absorption, extinction, and refractive indices were determined. Next, the conductivity in the THz range was calculated from the complex permittivity function. By fitting the conductivity characteristics to the Drude–Smith model, effective charge carrier parameters such as concentration and relaxation time were determined. The results obtained from THz-TDS spectroscopy were compared with those obtained from Raman spectroscopy and SEM imaging. This allowed us to verify whether the differences between the materials were evident in the results from the measurement techniques used.

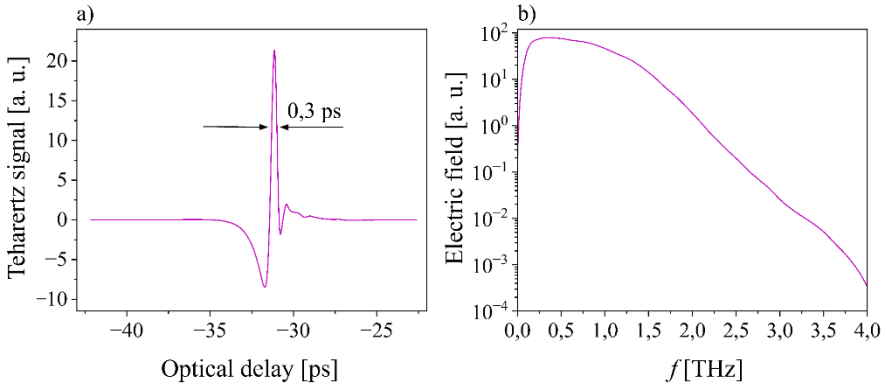


Figure 1. a) An example of a terahertz signal in the time domain and b) the signal's spectrum in the frequency domain after a Fourier transform

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Isotopically pure ^{10}BN: optical properties and applications in neutron detectors

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Boron nitride (BN) is a new emerging semiconductor material that is promising for many applications due to its high thermal and chemical stability. sp^2-bound BN polytypes: hexagonal BN (hBN) and rhombohedrical BN (rBN) combine wide energy bandgap of approximately 6 eV [1] with dielectric properties and thermic stability enabling the suitable platforms for various heterostructures [2] and deep ultraviolet devices [3].

Another interesting property of BN is ^{10}B's exceptionally high cross section for absorption of thermal neutrons ($\sigma \approx 3840 \pm 9$ b) [4] allowing ^{10}BN to be used in high efficiency neutron detectors [5]. Interaction of ^{10}B nuclei with thermal neutron leads to one of two reactions:

$$^{10}\mathrm{B} + {}^{1}\mathrm{n} \rightarrow {}^{7}\mathrm{Li}^{*} + {}^{4}\alpha^{*},\ \mathrm{p} = 94\%$$

$$^{10}\mathrm{B} + {}^{1}\mathrm{n} \rightarrow {}^{7}\mathrm{Li} + {}^{4}\alpha,\quad \mathrm{p} = 6\%$$

where the charged products could ionize BN itself, creating electrical impulses or scintillation light or could be detected outside of the BN crystal, which in such a case serves as a conversion layer.

In this work we present results of investigation of a thermal neutron detector consisting of an isotopically pure, MOVPE grown, ^{10}BN conversion layer paired with a commercial photodiode in a role of an α-particles detector. Detector dimensions has been optimized based on calculations of neutron and charged particles interactions with BN and photodiode material. Our detector design has been tested with Pu-Be thermal neutron source, showing a promising increase of signal intensity in energy range corresponding to kinetic energies of Li nuclei and α - particles.

Possible development of scintillator-like neutron ^{10}BN detectors utilizing secondary signals provokes a question how does ^{10}BN optical properties differ from those of natural boron BN. In order to investigate potential differences, photoluminescence (PL) and Raman spectroscopy measurements has been conducted. These measurements revile change of phonon frequencies induced by different mass of ^{10}B. Moreover, a slight shift (about 2 meV) in PL energies of the carbon dimer center between pure ^{10}BN and natural isotopic composition BN was observed in hBN and rBN polytypes.

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Development of a Polarization Modulation Infrared Reflection-Absorption Spectroscopy (PM-IRRAS) setup for model studies of catalytic reactions over single-atom catalysts

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Single-Atom Catalysts (SACs) exhibit remarkable catalytic performance thanks to their unique electronic properties related to the finite size of the active species, as well as charge transfer effects between the isolated metal atoms and the supporting substrate [1,2]. Due to the relatively low number of active sites at the catalyst's surface, model studies on SACs require state-of-the-art scientific techniques with extreme sensitivity. Polarization Modulation Infrared Reflection-Absorption Spectroscopy (PM-IRRAS) has emerged as a powerful analytical method for non-destructive, in situ characterization of ultrathin films, molecular monolayers and adsorption processes at solid-gas interfaces [3,4], being ideal for the studies of SACs.

Our group is developing a PM-IRRAS setup for model operando studies of greenhouse gas (N_2O, CO_2) conversion reactions over SACs based on Fe atoms embedded in epitaxial graphene on Ru(0001). The system will allow working at elevated temperatures and in gas pressures ranging from ultra-high vacuum (UHV) to 1 bar. The construction is based on a state-of-the-art all-vacuum Fourier-Transform Infrared (FTIR) spectrometer characterized by a superior resolution of 0.07 cm^{-1} and equipped with an ultrasensitive Mercury Cadmium Telluride (MCT) detector. The instrument also has the possibility to collect 40 spectra per second, allowing investigation of time-dependent processes, such as catalytic reactions.

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The studies are financially supported by the National Science Centre of Poland through the SONATA BIS project No. 2023/50/E/ST3/00704.

Exploring the Resolution Limit of Raman Thermometry

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Temperature is a crucial parameter in many applications and measurements, such as heat dissipation in nanoelectronic devices or thermal property characterization. Therefore, it is essential to determine the resolution limit of each method of temperature extraction. Here, we explore the limits of Raman thermometry, which can be used to measure a wide range of bulk and nanomaterials and can be particularly useful in opto-thermal Raman method. [1]

In this work, we look for the most effective approach to temperature measurement using Raman thermometry. Different temperature-dependent parameters of Raman spectra are examined, such as peak position shift and the anti-Stokes to Stokes intensity ratio. We find that the temperature resolution calculated from the Raman peak position shift provides the most accurate approach to temperature determination and it was observed that performing a series of measurements and statistically determining the temperature yields resolution values up to one order of magnitude lower. [2]

This short communication present different approaches to determining temperature resolution using Raman thermometry and demonstrate the importance of statistical measurements.

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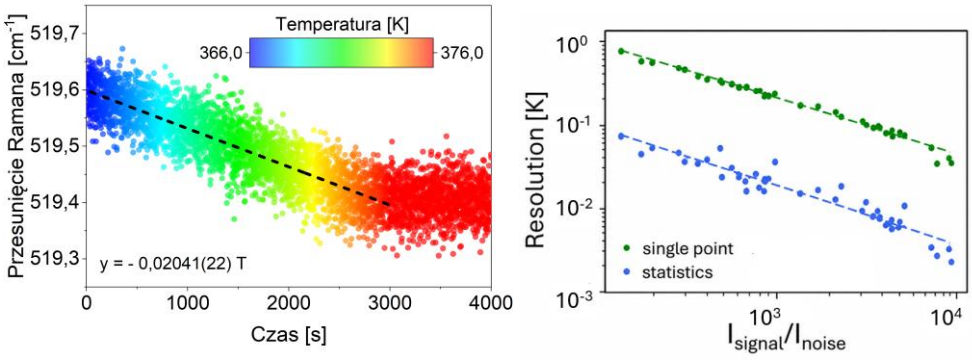


Figure 1. (a) dependence of the change in peak position as a function of temperature; (b) comparison of different methods for determining temperature resolution

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The authors acknowledge financial support from the Polish National Science Centre under the OPUS grant No. 2025/57/B/ST11/02260.