

# GRAPHENE & 2D Mat

POLISH CONFERENCE



9<sup>th</sup> Polish Conference

„Graphene and other 2D materials”

## Book of Abstracts

*Poznań, 8-10 September 2024*

*[graphene2d.web.amu.edu.pl](http://graphene2d.web.amu.edu.pl)*

HONORARY PATRONAGE



Polish Vacuum Society

NanoBioMedical Centre  
Adam Mickiewicz University  
in Poznań



## Contents

Scientific Committee .....	3
Organizing Committee.....	5
Chairs of the sessions.....	7
Exhibitors.....	9
Plenary & Invited Speakers .....	12
Programme.....	14
List of posters presentations .....	20
Abstracts .....	22
List of Participants .....	94

# GRAPHENE & 2D Mat

POLISH CONFERENCE



## Scientific Committee

**Maria Augustyniak-Jabłokow**, Polish Academy of Sciences, Poznań, Poland

**Leszek Bryja**, Wrocław University of Science and Technology, Wrocław, Poland

**Joanna Jadczyk**, Wrocław University of Science and Technology, Wrocław, Poland

**Agnieszka Jastrzębska**, Warsaw University of Technology, Warsaw, Poland

**Ryszard J. Kaleńczuk**, West Pomeranian University of Technology, Szczecin, Poland

**Piotr Kossacki**, University of Warsaw, Warsaw, Poland

**Paweł J. Kowalczyk**, University of Łódź, Łódź, Poland

**Mikołaj Lewandowski**, Adam Mickiewicz University in Poznań, Poland

**Sebastian Maćkowski**, Nicolaus Copernicus University in Toruń, Toruń, Poland

**Jacek A. Majewski**, University of Warsaw, Warsaw, Poland

**Ewa Mijowska**, West Pomeranian University of Technology, Szczecin, Poland

**Andrzej Olszyna**, Warsaw University of Technology, Warsaw, Poland

**Arkadiusz Wójs**, Wrocław University of Science and Technology, Wrocław, Poland

**Andrzej Wysmolek**, University of Warsaw, Warsaw, Poland

**Mariusz Zdrojek**, Warsaw University of Technology, Warsaw, Poland

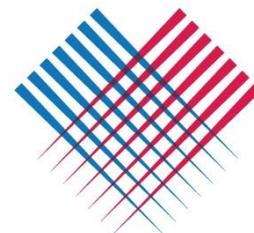
GRAPHENE  
& 2D Mat  
POLISH CONFERENCE



# Organizing Committee

**Adam Mickiewicz University**

**NanoBioMedical Centre**



**Mikołaj Lewandowski (Chairman)**

Anna Lewandowska-Andrałojć

Arkadiusz Ptak

Anna Dyrdał

Weronika Andrzejewska

Błażej Scheibe

Marta Woźniak-Budych

Nataliya Babayevska

Mariya V. Dobrotvorska

Szymon Murawka

Alicja Joras

Anna Maciejewska

Roksana Markiewicz

GRAPHENE  
& 2D Mat  
POLISH CONFERENCE



# **Chairs of the sessions**

**Anna Dyrdał**, Adam Mickiewicz University in Poznań, Poland

**Tomasz Kosmala**, University of Wrocław, Wrocław, Poland

**Piotr Kossacki**, University of Warsaw, Warsaw, Poland

**Paweł J. Kowalczyk**, University of Łódź, Łódź, Poland

**Mariusz Krawiec**, Maria Curie-Skłodowska University

**Mikołaj Lewandowski**, Adam Mickiewicz University in Poznań, Poland

**Anna Lewandowska-Andrałojć**, Adam Mickiewicz University in Poznań, Poland

**Sebastian Maćkowski**, Nicolaus Copernicus University in Toruń, Toruń, Poland

**Jacek A. Majewski**, University of Warsaw, Warsaw, Poland

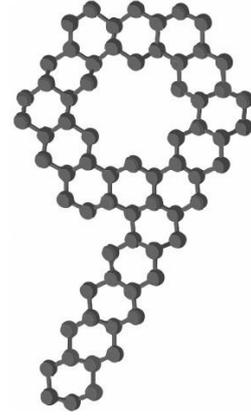
**Błażej Scheibe**, Adam Mickiewicz University in Poznań, Poland

**Andrzej Wysmolek**, University of Warsaw, Warsaw, Poland

**Mariusz Zdrojek**, Warsaw University of Technology, Warsaw, Poland

**Ryszard Zdyb**, Maria Curie-Skłodowska University

GRAPHENE  
& 2D Mat  
POLISH CONFERENCE



# Exhibitors



**UNI-EXPORT**  
Instruments Polska

# SPECSGROUP

TECHNO  LUTIONS  
solutions  
for  
sci-tech

TECHNOLUTIONS SP. Z O.O.  
UL. WIEJSKA7  
99-400 ŁOWICZ



Atomic Force Microscopy (AFM) aka Scanning Probe Microscopy (SPM) is high-resolution method of imaging and measuring surface structures in three dimensions. The surface structure and its properties are mapped using a microprobe, most often made of silicon or silicon nitride, interacting with the surface of the sample using a small probetip with a diameter of 1 to several or several dozen nanometers (10-9 m).

Atomic Force Microscopy is commonly used in:

- Imaging of the semiconductor substrates, heterostructures, 2D materials,
- Mapping properties of semiconductor materials,
- Imaging of magnetic domains distribution and its changes within the external magnetic field,
- Study of the electrochemical properties (i.e C-V curves, deposition or reduction of the sample surface),
- Polymers and biopolymers imaging with enabled at molecular resolution.

Atomic force microscopy also enables the measurement of point interactions between molecules or individual structures (e.g. intercellular interactions).

Currently, the development and improvement of Scanning Probe Microscopy is carried out, among the automation of measurements, enabling dynamic surface studies, by increasing the speed of scanning without losing the quality of images, and making the method more intuitive and user-friendly, by making AFM equipment “smarter” and more automated.

Technolutions sp. z o.o. provides the Atomic Force Microscopes from Park Systems (Suwon, South Korea) and AFM-in-SEM scanning modules from Nenovision (Brno, Czech Republic).

At our booth, we will present the universal Park Systems NX7 atomic force microscope, enabling scanning of samples in the range of 50um x 50um x 15um. The microscope's design is based on decoupled XY and Z piezoelectric scanners, controlled and driven independently, and operating using low-noise closed feedback loop. Thanks to this solution, it is possible to operate the microscope using the Park System’s proprietary True Non-Contact™ that allows imaging the sample surface with the precise control of interaction between scanning probe and sample surface, that helps to prevent tip or sample wear and ensures the high – resolution imaging for a long time.

The presented microscope is equipped with the following measurement modes:

- PinPoint™ mode allowing for imaging of mechanical properties and imaging of mechanical and electrical properties simultaneously,
- electric modes: EFM, KPFM
- magnetic properties imaging mode.

For those interested, Technolutions sp. Z o. o. offers well-equipped laboratory, localized in Łowicz, Poland where more advanced measurements or studies can be performed.



GRAPHENE  
& 2D Mat  
POLISH CONFERENCE



**Plenary & Invited  
Speakers**

# Plenary Speakers

**Costas Galiotis**

FORTH & University of Patras  
Greece

**Mikhail Katsnelson**

Radbound University Nijmegen  
The Netherlands

# Invited Speakers

**Anika Schlenhoff**

University of Münster, Germany

**Semir El-Ahmar**

Poznań University of Technology, Poland

**Tomasz Kosmala**

University of Wrocław, Poland

**Włodzimierz Jaskólski**

Nicolaus Copernicus University in Toruń, Poland

**Piotr Kossacki**

University of Warsaw, Poland

**Klaas-Jan Tielrooij**

Eindhoven University of Technology, The Netherlands

**Adam Rycerz**

Jagiellonian University in Kraków, Poland

**Chris Van Haesendonck**

KU Leuven, Belgium

**Luca Vattuone**

University of Genoa, Italy

**Luca Gregoratti**

Elettra Sincrotrone Trieste, Italy

**Viera Skákalová**

Slovak Academy of Sciences in Bratislava, Slovakia

**Paweł J. Kowalczyk**

University of Łódź, Poland

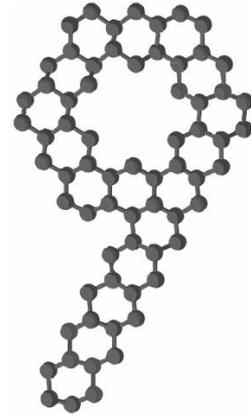
**Thomas Vasileiadis**

Adam Mickiewicz University in Poznań, Poland

**Patryk Florczak**

Adam Mickiewicz University in Poznań, Poland

GRAPHENE  
& 2D Mat  
POLISH CONFERENCE



# Programme

**SUNDAY 08.09.2024**

<b>FOR YOUNG RESEARCHERS WHO HAVE REGISTERED FOR THE WORKSHOPS</b>	
<b>13:50</b>	Get together in front of the “Entrance C” of the Faculty of Physics AMU
<b>14:00–15:30</b>	<b>Workshops part 1</b>
	<p><b>Group 1</b> – Atomic Force Microscopy (AFM) workshop pt. 1 organized by <i>Technolutions</i>, Room 13, Faculty of Physics AMU</p> <p><b>Group 2</b> – Ultra-high Vacuum/Scanning Tunneling Microscopy/X-ray Photoelectron Spectroscopy (UHV/STM/XPS) workshop pt. 1 organized by <i>PREVAC</i> and <i>www.surface-science.pl</i>, Room 14, Faculty of Physics AMU</p>
<b>15:30–16:00</b>	<b>BREAK</b>
<b>16:00–17:30</b>	<b>Workshops part 2</b>
	<p><b>Group 1</b> – AFM workshop pt. 2 organized by <i>Technolutions</i>, Room 13, Faculty of Physics AMU</p> <p><b>Group 2</b> – UHV/STM /XPS workshop pt. 2. organized by <i>www.surface-science.pl</i>, NanoBioMedical Centre AMU</p>
<b>FOR ALL PARTICIPANTS OF THE CONFERENCE</b>	
<b>17:30–18.30</b>	<b>Registration</b> in front of Prof. Stefan Jurga’s Auditory of the NanoBioMedical Centre AMU
<b>18:00–20:00</b>	<b>Reception</b> , Prof. Stefan Jurga’s Auditory of the NanoBioMedical Centre AMU

**MONDAY 09.09.2024**

<b>Venue: Faculty of Physics, Uniwersytetu Poznańskiego 2, Poznań</b>		
<b>8:00–14:30</b>	<b>Registration</b>	
<b>HALL A</b>		
<b>8:45–9:00</b>	<b>Opening Ceremony</b>	
<b>9:00–9:45</b>	<b>Costas Galiotis</b> <i>(Plenary Lecture)</i>	<i>Enhancing stress transfer in graphene-based composites: challenges &amp; innovations</i>
<b>9:45–9:50</b>	<i>(time to move between lecture halls)</i>	
<b>HALL A</b>		
<b>9:50–10:25</b>	<b>Paweł J. Kowalczyk</b> <i>(Invited Lecture)</i>	<i>2D Materials: path toward new phenomena</i>
<b>10:25–10:40</b>	Konrad Wilczyński	<i>Temperature-dependent anharmonicity in MoS<sub>2</sub> and MoS<sub>2</sub>/graphene structures: revisiting the impact of strain and interlayer interaction</i>
<b>10:40–10:55</b>	Subrahmanyam Bandaru	<i>Strain-induced effects in the electronic structure of thin layers of ScB.</i>
<b>HALL B</b>		
<b>9:50–10:25</b>	<b>Viera Skákalová</b> <i>(Invited Lecture)</i>	<i>Novel two-dimensional materials synthesized in graphene oxide under ambient conditions: atomic structure and properties</i>
<b>10:25–10:40</b>	Łukasz Majchrzycki	<i>Influence of graphene oxide thermal reduction on its properties in nanoscale</i>
<b>10:40–10:55</b>	Julia Czarnecka	<i>Instrumentation development towards a large-area, defect-free 2D materials synthesis and transfer</i>
<b>10:55–11:25</b>	<b>Coffee Break</b>	
<b>HALL A</b>		
<b>11:25–12:00</b>	<b>Luca Vattuone</b> <i>(Invited Lecture)</i>	<i>Graphene/Ni(111): adsorption and reactions under cover</i>
<b>12:00–12:15</b>	Piotr Radomski	<i>Transition metals vs. chalcogens: the impact on NO<sub>x</sub> adsorption on MoS<sub>2</sub>, MoSe<sub>2</sub> and WS<sub>2</sub> transition-metal dichalcogenides</i>
<b>12:15–12:30</b>	Klaudia Toczek	<i>Heterostructures based on bismuthene and van der Waals substrates as protection of 2D materials against oxidative degradation</i>
<b>12:30–12:45</b>	<b>SPECS</b> <i>Presentation of products</i>	
<b>12:45–13:00</b>	Przemysław Przybysz	<i>Heterostructure bilayer graphene and hBN – DFT calculation of the interactions between layers</i>
<b>13:00–13:15</b>	Paweł Wojciechowski	<i>Chemical functionalization of silicene on Au/Si(111) heterostructures</i>
<b>HALL B</b>		
<b>11:25–12:00</b>	<b>Adam Rycerz</b> <i>(Invited Lecture)</i>	<i>Possible strain-induced Mott transition in graphene and nanoscale Aharonov-Bohm effect in carbon nanotubes</i>
<b>12:00–12:15</b>	Lena Miler	<i>Temperature influence on direct and indirect bandgap transitions in aluminum alloyed boron nitride</i>
<b>12:15–12:30</b>	Piotr Pigoń	<i>Transport properties of a topological insulator sandwiched between ferromagnetic layers</i>

12:30–12:45	Maciej Chrobak	<i>Magnetotransport in nonstoichiometric and Mn-doped Bi<sub>2</sub>Te<sub>3</sub> 2D flakes</i>
12:45–13:00	Maciej Szyszko	<i>Computational analysis of two-dimensional alloy based systems</i>
13:00–13:15	Mirali Jafari	<i>Effect of Fe-doping on VS<sub>2</sub> monolayer: a first-principles study</i>
13:15	<b>Conference Photo</b>	
13:15–14:15	<b>Lunch</b>	
<b>HALL A</b>		
14:15–14:50	<b>Anika Schlenhoff</b> <i>(Invited Lecture)</i>	<i>Using image-potential states as local probes for magnetic Gr-hybrid systems</i>
14:50–15:25	<b>Klaas-Jan Tielrooij</b> <i>(Invited Lecture)</i>	<i>Heat transport in quantum materials with a cool twist</i>
15:25–15:40	Uni-Export Instruments	<i>Presentation of products</i>
15:40–15:55	Levan Chotorlishvili	<i>Magnetoelectric fractals, magnetoelectric parametric resonance and Hopf bifurcation</i>
15:55–16:10	Marcin Kurpas	<i>Spin mixing parameter as an indicator of Ising type-II pairing</i>
<b>HALL B</b>		
14:15–14:50	<b>Piotr Kossacki</b> <i>(Invited Lecture)</i>	<i>Ultrafast dynamics of excitons in monolayers of semiconductor TMDs</i>
14:50–15:25	<b>Thomas Vasileiadis</b> <i>(Invited Lecture)</i>	<i>Optomechanics of time-varying plasmonic-semiconducting nanomembranes</i>
15:25–15:40	Jan Kossacki	<i>Raman optical activity of the charge density wave-related phonon modes in 2H-TaSe<sub>2</sub> – a study by Raman scattering</i>
15:40–15:55	Marta Pelc	<i>GRANAD – framework and code for optoelectronic properties of low-dimensional structures</i>
15:55–16:10	Piotr Maksymiuk	<i>Raman studies of homoepitaxial hBN grown by MOVPE on isotopically-pure h<sup>10</sup>BN exfoliated flakes – PCA analysis</i>
16:30–19:30	<b>Poster Session &amp; Conference Barbecue</b>	

**TUESDAY 10.09.2024**

<b>Venue: Faculty of Physics, Uniwersytetu Poznańskiego 2, Poznań</b>		
<b>HALL B</b>		
<b>9:00–9:45</b>	<b>Mikhail I. Katsnelson</b> <i>(Plenary Lecture)</i>	<i>Structural commensurability and incommensurability in twisted van der Waals systems</i>
<b>9:45–9:50</b>	<i>(time to move between lecture halls)</i>	
<b>HALL A</b>		
<b>9:50–10:25</b>	<b>Luca Gregoratti</b> <i>(Invited Lecture)</i>	<i>Scanning photoelectron spectromicroscopy: from static to operando studies of 1D- and 2D-materials</i>
<b>10:25–10:40</b>	Aleksandra Nadolska	<i>Investigation of nanoscale electrical properties of epitaxial MoO<sub>3</sub></i>
<b>10:40–10:55</b>	Magdalena Birowska	<i>Revealing anisotropic features in structurally isotropic MPX<sub>3</sub> monolayers</i>
<b>HALL B</b>		
<b>9:50–10:25</b>	<b>Semir El-Ahmar</b> <i>(Invited Lecture)</i>	<i>Exploring the limits of graphene's operation in extreme conditions imposed by the future energy industry</i>
<b>10:25–10:40</b>	Łukasz Grzegorzółka	<i>Impact of neutron irradiation on defect-related photoluminescence in layered boron nitride</i>
<b>10:40–10:55</b>	Jakub Cwynar	<i>Influence of DUV illumination on the properties of MOVPE grown boron nitride layers</i>
<b>10:55–11:25</b>	<b>Coffee Break</b>	
<b>HALL A</b>		
<b>11:25–12:15</b>	<b>Chris Van Haesendonck</b> <i>(Invited Scholarly Lecture)</i>	<i>Scanning tunneling microscopy and spectroscopy of nanostructures: from fundamentals to applications</i>
<b>12:15–12:30</b>	<i>PREVAC</i>	<i>Presentation of products</i>
<b>12:30–12:45</b>	Ireneusz Morawski	<i>Herringbone structures with variable periodicities as the effect of van der Waals Au-Au interactions observed in Au 1 ML on the Ru(0001) surface</i>
<b>12:45–13:00</b>	Weronika Andrzejewska	<i>Structure of monolayer iron nitride islands on Cu(001) exposed to ambient conditions</i>
<b>13:00–13:15</b>	Izabela Rogala	<i>Investigating polytypism in layered boron nitride using TEM Moiré patterns analysis</i>
<b>HALL B</b>		
<b>11:25–12:00</b>	<b>Patryk Florczak</b> <i>(Invited Lecture)</i>	<i>Electrochemical oxidation of natural graphite as new way of producing a wide range of graphene-based materials</i>
<b>12:00–12:15</b>	Karolina Filak-Mędoń	<i>Graphene-based nanocomposites for applications in radiation protection and thermal management</i>
<b>12:15–12:30</b>	Technolutions	<i>Presentation of products</i>
<b>12:30–12:45</b>	Karolina Pietrusewicz	<i>Transition metal-doped nickel phosphides on cellulose: efficient electrocatalysts for the oxygen evolution reaction</i>

12:45–13:00	Tomasz Kędzierski	<i>Lanthanoid sesquioxide ultrafine nanoparticles on graphene via general and novel approach of Ultrafast Redox Reaction and their performance as anodes in lithium-ion batteries</i>
13:00–13:15	Grzegorz Leniec	<i>Structural studies of borophene materials by Electron Paramagnetic Resonance technique</i>
13:15–14:15	<b>Lunch</b>	
<b>HALL A</b>		
14:15–14:50	<b>Włodzimierz Jaskólski</b> <i>(Invited Lecture)</i>	<i>On the robustness of gapless states in gated multilayer graphene</i>
14:50–15:05	Izabella Wojciechowska	<i>Proximity induced spin-orbit coupling phenomena in twisted graphene-based van-der-Waals heterostructures</i>
15:05–15:20	Paulina Jureczko	<i>Electronic and optical properties of twisted PtSe<sub>2</sub></i>
15:20–15:35	Wojciech Rudziński	<i>Spin waves in a TMD bilayer antiferromagnet</i>
<b>HALL B</b>		
14:15–14:50	<b>Tomasz Kosmala</b> <i>(Invited Lecture)</i>	<i>Revealing active sites and boosting catalytic performance in 2D materials for hydrogen evolution reaction</i>
14:50–15:05	Klaudia Maślana	<i>Morphological influence on the electrocatalytic efficiency of nickel phosphide and nanocarbon for water electrolysis</i>
15:05–15:20	Sanjay Sahare	<i>Role of MXenes to improve the air stability in perovskite solar cell</i>
15:20–15:35	Daria Baranowska	<i>Photoelectrochemical hydrogen evolution utilizing borophene/MoS<sub>2</sub> heterostructure</i>
<b>HALL A</b>		
15:35–15:50	<b>Closing Ceremony</b>	
16:00–17:00	<i>Visiting the laboratories of the NanoBioMedical Centre AMU</i>	

GRAPHENE  
& 2D Mat  
POLISH CONFERENCE



**List of posters  
presentations**

## LIST OF POSTERS

- P1. **A. Aligayev**, 2D materials catalysis: a multiscale quantum chemistry approach for hydrogen production from CH<sub>4</sub>, CO<sub>2</sub> purification, and gas splitting applications
- P2. **P. Radomski**, Demonstration of power of the boron-doped MoTe<sub>2</sub>: computational study of N<sub>2</sub>O, NO<sub>2</sub>, NO, N<sub>2</sub>, CO<sub>2</sub>, CO, O<sub>2</sub>, H<sub>2</sub>O, and H<sub>2</sub> adsorption
- P3. **M. J. Szary**, Toward high selectivity of sensor arrays: selectivity of gas detection on transition metal dichalcogenides
- P4. **M. Smirnova**, The role of MXene purification and ion intercalation processes in optimizing photocatalytic hydrogen production
- P5. **Y. Hua**, Graphene oxide modified zinc anode to improve cycle stability of zinc ion capacitor
- P6. **A. Leśniewicz**, Non-covalent interaction of meso-tetrakis(p-sulfonatophenyl) porphyrin with graphene oxide and reduced graphene oxide
- P7. **A. Kolman**, Nanohybrid systems of m-THPC with Pluronic P123 and graphene oxide: a promising approach for photodynamic cancer therapy
- P8. **M. Solovan**, Extreme radiation resistance of quasi-2D perovskite solar cells
- P9. **W. Krumplewski**, Development of sorption phases with reduced graphene oxide, multiwalled carbon nanotubes and heavy oil fly ash for TF-SPME microextraction and their use for the isolation of PAHs from aqueous matrices
- P10. **J. Olejnik** Comparison of the excitonic upconversion photoluminescence in MoSe<sub>2</sub> monolayers with a different doping level
- P11. **E. Żuberek**, Upconversion photoluminescence of a defect-bound exciton in hBN-encapsulated MoS<sub>2</sub> monolayers
- P12. **T. Kędzierski**, Biopolymers based paper coating with promoted grease resistivity, bio-degradable and mechanical properties
- P13. **K. Maślana**, Optimizing paper properties with various inorganic crosslinkers for enhanced filler retention
- P14. **P. Sać**, Fabrication and characterization of 2D heterostructure based on MoSe<sub>2</sub> and borophene
- P15. **M. Kurpas**, Proximity spin-orbit effects in hybrid 1D/2D heterostructures.
- P16. **J. Woronowska**, Photo-electrochemical characterization of 2D heterostructure based on MoSe<sub>2</sub> and borophene
- P17. **K. Gałazka**, Machine Learning assisted approach for prediction of the g factors of TMDs heterobilayers
- P18. **Q. Yang**, Refinement and optimization strategies for the transfer and hierarchical stacking of graphene films
- P19. **M. Gołębiowski**, Synthesis and characterization of free-standing-like antimonene monolayer on silicon
- P20: **M. Pelc**, Atoms near graphene nanoantennas: interplay of optical coupling and electron tunneling
- P21: **I. Morawski**, Herringbone structures with variable periodicities as the effect of van der Waals Au-Au interactions observed in Au 1 ML on the Ru(0001) surface

GRAPHENE  
& 2D Mat  
POLISH CONFERENCE



# Abstracts

## Enhancing stress transfer in graphene-based composites: challenges & innovations

C. Galiotis<sup>1,2</sup>

<sup>1</sup>*Institute of Chemical Engineering Sciences, Foundation for Research & Technology–  
FORTH, Patras, Greece*

<sup>2</sup>*Department of Chemical Engineering, University of Patras, Patras, Greece*

Given its superior mechanical behaviour, combined with exceptional electrical and thermal properties, graphene has become the ideal candidate for lightweight, high-strength and multi-functional composites. So far, only graphene in the form of powders has been adopted for the production of nanocomposites for large scale applications. However, the mechanical performance of such systems is generally far below the expectations, and a lot of research has been performed to shed light onto the mismatch between theoretical predictions and observed behaviour [1], highlighting that the performance and reliability of graphene-based systems are often limited by the interfacial properties between graphene and the substrate material or surrounding matrix [2].

Due to the microscopic size of the flakes, the interfacial properties of graphene-based composites cannot be directly measured by using conventional micromechanical testing methods (e.g. fiber pullout, fragmentation, and micro-debonding test). In the last decades, our group has pioneered a unique and precise method based on the application of in-situ Raman spectroscopic mapping to investigate the mechanical behaviour of graphene flakes under both tension and compression [3-7]. In analogy with other carbon-based materials, graphene presents a well-defined Raman spectrum and its characteristic peaks are found to shift under the imposition of a mechanical loading. It has been demonstrated that these stress-induced Raman band shifts can be used to monitor the stress/ strain in graphene and that this can be employed for the study of the interfacial micromechanics in model composite specimens. Using this technique, the stress transfer and the efficiency of reinforcement of graphene have been found to be affected by several factors, such as the lateral size of the flake, the presence of doping, the number of layers, the morphology and the geometry of graphene. Moreover, the technique can be exploited to monitor the stress field around a notch in composites structures, as well. In this talk, a comprehensive analysis of the above issues is given, and key parameters towards the design and production of high-performance and durable composites are delineated, with emphasis on our recent progresses in the field.

### References

- [1] C. Pavlou *et al.*, Nature Comms 12 (2021) 4655.
- [2] A. C. Manikas *et al.*, Nanoscale 11 (2019) 14354.
- [3] G. Tsoukleri *et al.*, Small 5 (2009) 2397.
- [4] O. Frank *et al.*, ACS Nano 4 (2010) 3131.
- [5] C. Androulidakis *et al.*, Scientific Reports 4 (2014) 5271.
- [6] G. Anagnostopoulos *et al.*, ACS applied materials & interfaces 7 (2016) 4216.
- [7] C. Androulidakis *et al.*, Nanoscale Advances 1 (2019) 4972

### Acknowledgments

This work has been supported by the European Research Council (ERC Advanced Grant 2013) via project no. 321124 (“Tailor Graphene”) and by the EU Graphene Flagship funding via project nos. 604391 (Graphene Flagship), 696656 (GrapheneCore1), 785219 (GrapheneCore2), 881603 (GrapheneCore3).

## 2D Materials: path toward new phenomena

P. J. Kowalczyk

*University of Lodz, Faculty of Physics and Applied Informatics,  
Pomorska 149/153, 90-236 Lodz, Poland*

Recently, growing interest in 2D materials is observed initiated by exfoliation of graphene followed by investigations of silicane, germanene and stanene all located in 14th group of periodic table. Elements located in 15th group are also capable to crystalize in 2D form in layered A17 structure (black phosphorus structure,  $\alpha$ -form). The widely investigated  $\alpha$ -phosphorene is best known example, however,  $\alpha$ -arsenene,  $\alpha$ -antimonene,  $\alpha$ -bismuthene and  $\alpha$ -bismuth antimonidene can be synthesized. Interestingly, Sb and Bi can also form stable hexagonal form i.e.  $\beta$  phase based on A7 structure (blue phosphorus). After successive synthesis of these materials we investigated their properties and over years we found number of interesting phenomena including unpinned Dirac states [1], nonsymorphic symmetries leading to formation of Dirac points [2], possible topologically protected edge states [3] and recently superlubricity and signatures of Levy flights in spontaneous diffusion of Bi on graphite [4].

The other group of 2D materials is based on transition metal dichalcogenide (TMDC) compounds. From this large group we will focus on TaS<sub>2</sub> and WTe<sub>2</sub> and their hybrids with graphene. These preliminary research show presence of variety of moire patterns indicating great platform for twistroinics. We will also briefly discuss ageing and laser induced modification of MoTe<sub>2</sub>, WTe<sub>2</sub> and BiTeCl.

Finally, graphene can serve as electrode in many applications. To use it in photovoltaics its work function (WF) has to be substantially increased. We started series of experiments with 2D oxide MoO<sub>3</sub> growth [4, 5] which allowed us to tune graphene WF and create first working OLED in Poland.

All these experiments are conducted using surface sensitive techniques including SPM and ARPES. Some of the experiments were conducted with LEEM/PEEM and STXM which are available only at synchrotron facilities.

### References

- [1] Q. Lu *et al.*, Nat. Comm. 13 (2022) 4603
- [2] P.J. Kowalczyk *et al.*, ACS Nano 14 (2020) 1888
- [3] S. Salehitaleghani *et al.*, 2D Mat. 10 (2022) 15020
- [4] M. Le Ster *et al.*, arXiv 2406.16709, <https://doi.org/10.48550/arXiv.2406.16709>
- [5] D. Kowalczyk *et al.*, 2D Mat. 8 (2021) 25005
- [6] D. Kowalczyk *et al.*, ACS Appl. Mat. Int. 14 (2022) 44506

### Acknowledgments

This work was possible thanks to National Science Centre, Poland under projects: 2020/37/B/ST5/03929 (OLED), 2019/35/B/ST5/03956 (Bi, Sb), 2018/31/B/ST3/02450 (TMDC)

## Temperature-dependent anharmonicity in MoS<sub>2</sub> and MoS<sub>2</sub>/graphene structures: revisiting the impact of strain and interlayer interaction

K. Wilczyński, A. P. Gertych and M. Zdrojek

*Faculty of Physics, Warsaw University of Technology, Koszykowa 75, 00-662 Warsaw, Poland*

In this work, we study the thermal expansion and phonon anharmonicity in popular two-dimensional structures – MoS<sub>2</sub> monolayers and MoS<sub>2</sub>/graphene heterostructures – using first-principles DFT simulations and a rigorous quantum-mechanical description of anharmonic crystals [1]. Our models provide a complete explanation of anharmonicity in those systems with exceptional agreement to available Raman experiments – exceeding the state-of-the-art simulations [2]. The accuracy of our models originates from the proper inclusion of all key anharmonic factors: the thermal expansion of all geometrical degrees of freedom (*i.e.*, all in-plane and out-of-plane dimensions) and the amplitude dependence of phonon frequencies due to three- and four-phonon interaction processes. Two of the factors considered in our work – the thermal expansion of the MoS<sub>2</sub> monolayer’s thickness and four-phonon interaction processes – are commonly skipped in the literature. However, their impact on phonon frequencies appears to be of the same order as of the other factors, so they must be addressed. In particular, the expansion of the MoS<sub>2</sub> monolayer’s thickness is crucial when describing the impact of external strains, as any reduction in the in-plane dimension of the monolayer involves an increase in its thickness – indirectly affecting phonon frequencies. Besides, the four-phonon processes are affected by interlayer interactions, leading to differences in the slopes  $d\omega/dT$  of temperature-dependent phonon frequencies in mono- and multi-layered systems. We also highlight the impact of interactions between the layers in the MoS<sub>2</sub>/graphene heterostructure on its thermal expansion, especially in the in-plane direction. In that case, the graphene layer acts like a substrate – with an uncommon negative thermal expansion.

Besides, our contribution provides a significant improvement in the methodology of studying phonon anharmonicity in the solid-state. Our approach, based on the inclusion of “frozen phonons” [3, 4] in the structure (*i.e.*, enforcing a non-zero coordinate of one phonon mode), provides efficient calculation of crucial 3<sup>rd</sup>- and 4<sup>th</sup>-order Taylor expansion coefficients of the interatomic potential. We also highlight the importance of applying symmetry conditions such as the rotational invariance rule, which affects low-frequency phonon dispersions and final phonon anharmonicity, especially in two-dimensional structures. Overall, our work sheds new light on future studies of phonon anharmonicity in 2D materials, also on substrates.

### References

- [1] R. A. Cowley, Rep. Prog. Phys. 31 (1968) 123.
- [2] S. Sarkar et al., Phys. Rev. B 101 (2020) 205302.
- [3] K. Wilczyński *et al.*, J. Phys. Chem. C 127 (2023) 20870.
- [4] K. Wilczyński *et al.*, Acta Materialia 240 (2022) 118299.

### Acknowledgments

Research was funded by the Warsaw University of Technology within the Excellence Initiative: Research University (IDUB) programme. Within this programme, “Young” grants were realized by K.W. & M.Z. and by A.G. We also acknowledge the usage of computer cluster DWARF at Warsaw University of Technology supported by the Polish National Science Center (NCN) under Contracts No. UMO-2017/26/E/ST3/00428 and UMO-2017/27/B/ST2/02792.

## Strain-induced effects in the electronic structure of thin layers of ScB.

S. Bandaru<sup>1</sup>, M. Birowska<sup>1</sup>, M. Rybak<sup>1</sup> and A. Jastrzębska<sup>2</sup>

<sup>1</sup>*Faculty of Physics, University of Warsaw, Pasteura 5, PL-02093 Warsaw, Poland,*

<sup>2</sup>*Warsaw University of Technology, Faculty of Materials Science and Engineering, 02-507 Warsaw, Wołoska 141, Poland*

MBenes, an emerging member of the two-dimensional (2D) materials family, are attracting significant attention due to their unique mechanical and electronic properties, which make them suitable for various applications [1, 2]. However, the intrinsic metallic nature of pristine MBenes can pose challenges for applications in optics that involve photon absorption, emission, and electronics. In semiconductor materials, the bandgap is the most crucial parameter, and significant effort is dedicated to finding new nanomaterials with a wide range of bandgaps. Therefore, the MBene family, as a new member of the flatland materials, appears to be a promising candidate with its diverse symmetries and structures [1-3].

Although MBenes generally exhibit metallic behavior, they can be tuned to become semiconducting through band engineering techniques such as surface functionalization and straintronics. We investigated various crystal symmetries of ScB MBene and examined their structural and dynamic stability. Our results reveal that ScB with hexagonal symmetry is the most stable crystal phase. The electronic structures of ScB functionalized with O, F, OH, and H groups were examined, and band structure calculations reveal that ScB functionalized with O becomes semiconducting, with a bandgap of around 0.1 eV and 0.5 eV using DFT+U and the hybrid exchange-correlation functional HSE06, respectively. Furthermore, applying in-plane biaxial strain further enhanced the bandgap ScBO. This makes ScBO MBene advantageous for electronic, optical, and various other applications.

### References

- [1] V.G. Nair, et. al Two-dimensional MBenes: a Novel Member in the Flatland, *Advanced Materials*, March 2022
- [2] S. Bandaru, et. al Recent progress in thermoelectric MXene-based structures versus other 2D materials, *Applied Mat.Today* 34, 101902 (2023).
- [3] D. Bury, et. al Wet-chemical etching and delamination of MoAlB into Mo<sub>2</sub>B<sub>2</sub> MBene and its outstanding photocatalytic performance, *Adv. Funct. Materials* 33, (2023).

## Novel two-dimensional materials synthesized in graphene oxide under ambient conditions: atomic structure and properties

V. Skákalová<sup>1,2</sup>, P. Kotrusz<sup>1,2</sup>, K. Mustonen<sup>3</sup>, T.A; Bui<sup>3</sup>, M. Precner<sup>1</sup>, P. Hutár<sup>1</sup>, M. Hulman<sup>1,2</sup>, M. Orendáč<sup>4</sup> and M. Gmitra<sup>4</sup>

<sup>1</sup>*Institute of Electrical Engineering, Slovak Academy of Sciences, Bratislava (Slovakia),*

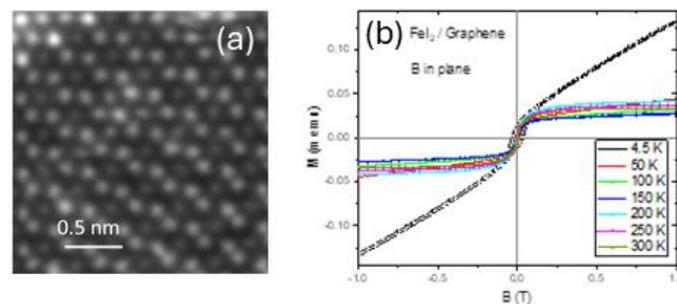
<sup>2</sup>*Danubia NanoTech, s.r.o. (Slovakia),*

<sup>3</sup>*University of Vienna, Faculty of Physics (Austria),*

<sup>4</sup>*Institute of Experimental Physics, Slovak Academy of Sciences, Košice (Slovakia),*

We have recently developed a simple chemical method SinGO (Synthesis in Graphene Oxide) that, under ambient conditions, can provide novel two-dimensional (2D) materials in a macroscopic scale [1]. The SinGO method opens an avenue to a new class of 2D magnetic and non-magnetic metal-iodides (2D-MI) encapsulated between graphene monolayers. Such vdW stacks would serve as a novel platform for nanotechnological devices in which 2D magnets hold spin whereas graphene as a conducting channel of Dirac electrons can guide the encoded relevant information. Noting that graphene spintronics has been aiming to exploit the extraordinary Dirac electronic properties but weak spin orbit-coupling limits its applicability for generating spin currents or spin torques. The proximity-induced spin-orbit coupling and exchange interactions in graphene-encapsulated 2D-MI magnets heterostructure might enable spin transport with unexplored yet physical mechanisms.

Here we will present the wide range characterization of 2D (magnetic and non-magnetic) metal-iodides encapsulated in graphene including their atomic structures (STEM), magnetization and electrical transport properties for possible applications.



**Figure 1.** (a). Scanning Transition Electron Micrograph of 2D FeI<sub>2</sub> atomic structure embedded between graphene layers (carbon contrast is too low to be visible), (b). Dependence of magnetization on magnetic field of 2D FeI<sub>2</sub> - graphene heterostructure.

### References

- [1] K. Mustonen et al., Toward Exotic Layered Materials: 2D Cuprous Iodide, *Advanced Materials* 34, 2106922 (2022).

### Acknowledgments

V.S. was supported by the V4-Japan Joint Research Program (BGapEng). Austrian Science Fund FWF (project no. P35912) and the Czech Science Programme Johannes Amos Comenius (project QM4ST, No. CZ.02.01.01/00/22\_008/0004572).

## **Influence of graphene oxide thermal reduction on its properties in nanoscale**

Ł. Majchrzycki, M. Weiss and A. Ptak

<sup>1</sup>*Institute of Physics, Faculty of Materials Engineering and Technical Physics, Poznan University of Technology, Piotrowo 3, 60-965 Poznan, Poland*

The surface's tribological properties are essential due to the high costs linked to wear on working surfaces. Therefore, significant efforts are directed towards reducing friction and surface wear. This is especially important in nano- and micromechanical systems where fluid lubricants cannot be used, making thin film coatings a desirable alternative [1]. One potential candidate for anti-wear coatings is graphene oxide (GO). GO's properties can be tailored through a reduction process, making it suitable for use as a thin film interface.

This study examines how low-temperature thermal reduction (90°C–150°C) affects GO's conductivity and tribological properties at the nanoscale. Conductive atomic force microscopy (C-AFM) was used to determine the temperature range needed to increase the GO's local conductivity. Additionally, friction force microscopy (FFM) and force spectroscopy (FS) provided data on adhesion force and friction force as a function of sliding velocity. The threshold temperature from these experiments consistently matched, suggesting a common source for the changes observed. All this data indicates that GO can serve as an interface coating with properties adjustable through simple low-temperature annealing.

### **References**

[1] M. Weiss *et al.*, Tribology International 162 (2021) 107133.

### **Acknowledgments**

This work was supported by the National Science Centre in Poland under Project No. 2020/37/B/ST8/02023 (OPUS-19) and the Ministry of Education and Science in Poland under Project No. 0512/SBAD/2320.

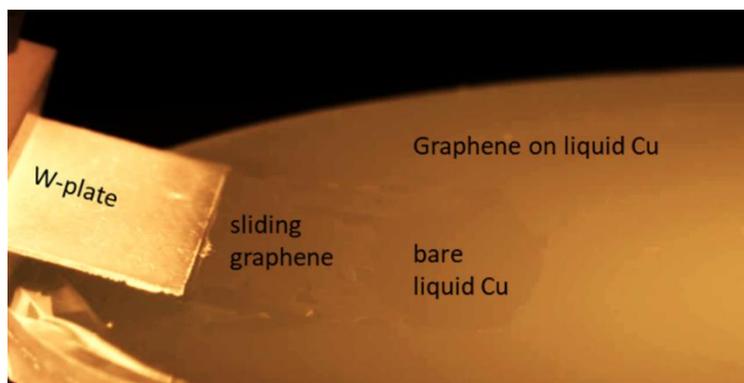
## Instrumentation development towards a large-area, defect-free 2D materials synthesis and transfer

J. Czarnecka and G. van Baarle

*Leiden Probe Microscopy (LPM), Kenauweg 21, 2331 BA Leiden, The Netherlands*

The synthesis and transfer of large-area, defect-free, and minimally contaminated 2D materials remain a challenge for many of their desired industrial applications. In this work, we present findings from the EU Horizon-funded DirectSepa project and its successor, 2D Engine, which focus on innovative methods for the growth and transfer of materials from single monolayers up to a few layers thick, some of which are unobtainable through equilibrium growth methods in bulk.

We introduce a custom-built chemical vapor deposition (CVD) reactor designed for in-situ monitoring of 2D material growth on liquid metal catalysts (LMCats) [1]. This reactor's optical monitoring system exploits emissivity differences between LMCats and the grown film, which we demonstrate on the example of liquid copper and copper covered with graphene. By analysing black body radiation intensity within the optical spectrum, our system provides sufficient contrast for real-time observation of graphene domain formation, ranging from 1 to 2000  $\mu\text{m}$  in size. Additionally, we extend our scope to other 2D materials, including GaN, AlN, and hBN, aiming to replicate our success with graphene. We also present results on the direct separation of grown materials from the liquid metal substrate. Central to this process is a specially designed robotic arm engineered for delicate handling and transfer of graphene layers without introducing defects. These advancements are expected to significantly impact the scalability and quality of 2D materials for industrial applications, particularly in the fields of (opto)electronics.



**Figure 1** Robotic-arm aided separation of graphene from the liquid copper substrate.

### References

[1] Saedi M, de Voogd J.M, Sjardin A., Manikas A., Galiotis C., Jankowski M., Renaud G., La Porta F., Konovalov O., van Baarle G. JC et al. 2020. Development of a reactor for the in-situ monitoring of 2D materials growth on liquid metal catalysts, using synchrotron x-ray scattering, Raman spectroscopy, and optical microscopy. Review of Scientific Instruments. 91(1) 013907.

## Graphene/Ni(111): adsorption and reactions under cover

L. Vattuone<sup>1,2</sup>

<sup>1</sup>*DIFI Università degli Studi di Genova, Via Dodecaneso33, 16146 Genova (Italy)*

<sup>2</sup>*IMEM-CNR Genoa Unit Via Dodecaneso33, 16146 Genova (Italy)*

We report here about experimental investigation of the chemistry of *single* layer graphene grown on Ni(111) (G/Ni(111)). When G/Ni(111) is exposed to gas phase molecules they can adsorb at the G surface or intercalate under G and possibly react at the Ni(111) surface. The former phenomenon is important for sensoristic application [1] while the latter discloses the possibility to use the confined space between G and the substrate as a nano-reactor where the activation barriers for several reactions are actively reduced [2].

In both cases the substrate can play a key role: while no CO adsorption indeed takes place for G/Cu, molecular chemisorption occurs for G/Ni(111) [3]. Even if under UHV conditions CO desorption off G/Ni(111) occurs between 150 and 200 K, we demonstrated by NAP-XPS experiments performed at Soleil synchrotron that a significant equilibrium coverage of CO *above* G can be present at room temperature if the CO pressure is increased to a few mbar [4].

These results indicate that the reactivity of G can be significantly affected by its interaction with the substrate.

This is not true only for CO but also for H<sub>2</sub>. In previous reports hydrogenation of G was obtained using atomic H [5] while hydrogenation of G using H<sub>2</sub> molecules was reported only at pressures larger than 10 bar or using vibrationally excited molecules.

We found recently that exposure to H<sub>2</sub> at a pressure of the order of 1 mbar leads to hydrogenation of  $\approx 6\%$  of carbon atoms in G/Ni(111). NAP-XPS experiments performed at the Swiss Light Source have shown also that the attainable H coverage is at least two times larger when both G and NiO are present.

This somewhat surprising results is explained by DFT calculations: the calculated H<sub>2</sub> dissociation barrier decreases indeed from more than 4 eV for free standing G to less than 2 eV for G/Ni(111); this barrier might be further reduced for strained graphene in presence of NiO.

It is well established that at near ambient pressure CO intercalation occurs causing a detachment of the G layer. In this confined space we observed formation of CO<sub>2</sub> via the Boudouard reaction (CO+CO  $\rightarrow$  CO<sub>2</sub> + C) catalyzed by the Ni(111) surface already at 340 K [5] at a pressure of a few mbar, i.e. significantly lower than previously reported [6].

### References

- [1] F. Schedin et al., Nat. Mater. 6 (2007) 652
- [2] Q. Fu and X. Bao, Chem. Soc. Rev. 46 (2017) 1847
- [3] M. Smerieri et al., ChemCatChem 7 (2015) 2328
- [4] R. Davì et al, Appl. Surf. Sci. 599 (2022) 154065
- [5] D. Lizzit et al. ACS Nano 13 (2019) 1828
- [6] W. Snoeck et al. Ind. Eng. Chem. Res. 41 (2002) 4252

### Acknowledgments

Soleil Synchrotron and PSI Swiss Light Source are acknowledged for beamtime allocation and support. MIUR (Italy) is acknowledged for funding in PRIN2017 KFMJ8E\_003, PRIN2022 2022LS74H2, PRIN-PNRR P20227XSAH. Graphene&2D Mat 9 is acknowledged for support.

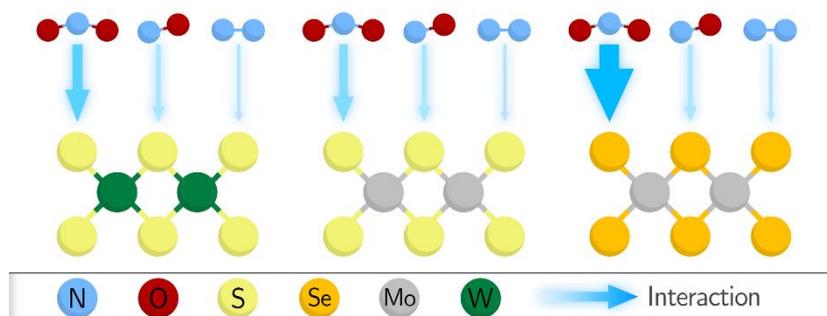
## Transition metals vs. chalcogens: the impact on NO<sub>x</sub> adsorption on MoS<sub>2</sub>, MoSe<sub>2</sub> and WS<sub>2</sub> transition-metal dichalcogenides

P. Radomski<sup>1</sup> and M. Szary<sup>2,\*</sup>

<sup>1</sup>*Institute of Materials Research and Quantum Engineering, Poznan University of Technology, ul. Piotrowo 3, 61-138 Poznan, Poland*

<sup>2</sup>*Institute of Physics, Poznan University of Technology, ul. Piotrowo 3, 61-138 Poznan, Poland*

The modern industrial sector generates considerable amounts of harmful gases, driving the need for advanced materials to detect these efficiently and reliably. Transition-metal dichalcogenides (TMDs) are an excellent example of such materials, notable for their high potential in sensing NO<sub>2</sub>. Although it is known that the adsorption of this hazardous molecule varies with the TMD composition, the specific roles of the transition metal and chalcogen types have not been previously compared. Additionally, other NO<sub>x</sub> compounds, *e.g.* NO and N<sub>2</sub>, interact much less with TMD sheets, a phenomenon that remains poorly understood. To illuminate this issue our study employs density functional theory (DFT) to investigate the adsorption processes of NO<sub>2</sub>, NO, and N<sub>2</sub> on monolayers of WS<sub>2</sub>, MoS<sub>2</sub>, and MoSe<sub>2</sub>. The findings reveal two key points: (i) the type of chalcogen has a more significant impact than the type of transition metal, and (ii) only molecules that act as acceptors relative to the TMD sheet can benefit from the interaction enhancement resulting from the composition of the layer. These insights could aid in designing devices capable of selective detection, addressing a well-known issue with semiconductor sensors.



**Figure 1.** Schematic representation of the differences in interaction between NO<sub>2</sub>, NO, and N<sub>2</sub> adsorbed on WS<sub>2</sub>, MoS<sub>2</sub>, and MoSe<sub>2</sub>.

### References

[1] P. Radomski and M. J. Szary, *Acta Materialia* 272 (2024) 119949.

### Acknowledgments

This work was supported by the Ministry of Education and Science in Poland (Grant No. 0512/SBAD/2320) within the project realized at the Institute of Physics, Poznan University of Technology. Computations reported in this work have been performed at Poznan Supercomputing and Networking Center (PSNC) under Grant No. 608.

## Heterostructures based on bismuthene and van der Waals substrates as protection of 2D materials against oxidative degradation

K. Toczek, M. Piskorski, M. Le Ster, I. Lutsyk, M. Rogala, P. Krukowski, P. Dąbrowski, R. Dunal, A. Nadolska, P. Przybysz, W. Ryś and P. J. Kowalczyk

*Department of Solid State Physics, Faculty of Physics and Applied Informatics, University of Lodz, Pomorska 149/153, 90-236 Lodz, Poland*

Two-dimensional materials are of growing interest due to their unique chemical, physical, electronic, and optical properties. [1] The less understood ones are in group 15th of the periodic table, and among them are those based on bismuth (Bi). It is a semi metal with minimal radioactivity. 2D-Bi exists in two crystallographic structures -  $\alpha$ -Bi (110) with a rectangular unit cell and  $\beta$ -Bi (111) with a hexagonal unit cell. [2]

It has been shown that 2D structures based on bismuth can be fabricated, at the edges of which unusual electron states appear to provide electron flow without electrical resistance, while the interior remains a semiconductor. [2,3] Thus, the fabrication of electronic devices based on Bi could contribute to advances in electronics, optoelectronics, spintronics and catalysis. However, Bi nanostructures are known to degrade rapidly in air. Therefore, it is extremely important to understand the growth and degradation pathways of this new material.

In this work, we will present the properties and morphology of heterostructures based on epitaxially grown bismuth and van der Waals materials - highly oriented pyrolytic graphite (HOPG) and hexagonal boron nitride (hBN).

The growth of bismuth thin films and heterostructures was done in ultra-high vacuum, X-ray photoelectron spectroscopy to analyze the chemical composition of metallic and oxidized surfaces. Raman spectroscopy (in an inert atmosphere) was also used to identify the oxidized phase on the sample surface, and the surface topography of the oxidized layers was also studied in the atmosphere using atomic force microscopy.

### References

- [1] H.G. Ali *et al.* J Energy Storage 73, 108980 (2023).
- [2] P.J. Kowalczyk *et al.* Surf Sci 605, 659–667 (2011).
- [3] S. Pinilla *et al.* Nature Reviews Materials 7, 717–735 (2022).

### Acknowledgments

The above research is supported by the National Science Center under the project no. 2019/35/B/ST5/03956.

## Heterostructure bilayer graphene and hBN - DFT calculation of the interactions between layers

P. Przybysz<sup>1,2</sup>, G. Feraco<sup>2</sup>, O. De Luca<sup>2</sup>, O. Zheliuk<sup>2</sup>, Y. Wang<sup>2</sup>, P. Dudin<sup>3</sup>, J. Avila<sup>3</sup>, J. Ye<sup>2</sup>, P. Dabrowski<sup>1</sup>, P. Krukowski<sup>1</sup>, M. Rogala<sup>1</sup>, M. Le Ster<sup>1</sup>, I. Lutsyk<sup>1</sup>, M. Piskorski<sup>1</sup>, R. Dunal<sup>1</sup>, W. Kozłowski<sup>1</sup>, P. Krempiński<sup>1</sup>, A. Nadolska<sup>1</sup>, W. Rys<sup>1</sup>, K. Toczek<sup>1</sup>, A. Grubišić-Čabo<sup>2</sup>, P. Rudolf<sup>2</sup>, J. Sławińska<sup>2</sup> and P. J. Kowalczyk<sup>1</sup>

<sup>1</sup> Faculty of Physics and Applied Informatics, University of Łódź, Pomorska 149/153, 90-236 Łódź, Poland

<sup>2</sup> Zernike Institute for Advanced Materials, University of Groningen, Nijenborgh 4, 9747 AG Groningen, The Netherlands

<sup>2</sup> Synchrotron SOLEIL, Université Paris-Saclay, Saint Aubin, BP 48, 91192 Gif sur Yvette, France

To study van der Waals heterostructures, we use theoretical calculations DFT (Density Functional Theory) and experimental ARPES (Angle-Resolved Photoemission Spectroscopy) to find interactions between layers and changes in band structure. The combination of these two methods gives us a greater understanding of the interactions occurring between heterostructure layers.

However, we are not always able to explain the complex band structure of the heterostructure using only DFT and ARPES. Therefore, in our research we used a third method, which is the simulation of an ARPES experiment via the Chinook program. In our work, we want to present the application of the Chinook program as a complement to the DFT and ARPES techniques to study interaction between bilayer graphene on hBN (hexagonal boron nitride). While we conducted ARPES experiments and DFT calculations for this heterostructure, certain regions of the experimental data remain unexplained solely by DFT. Thus, we performed simulated ARPES experiments to provide additional insights and explanations.

### Acknowledgments

This work was financially supported by the National Science Centre, Poland under projects 2018/30/E/ST5/00667 and 2018/31/B/ST3/02450.

The calculations were carried out on the Dutch national e-infrastructure with the support of SURF Cooperative (EINF-5312) and on the Hábrók high-performance computing cluster of the University of Groningen.

## Chemical functionalization of silicene on Au/Si(111) heterostructures

P. Wojciechowski, A. Stępnia-Dybala and M. Krawiec

*Institute of Physics, Maria Curie-Skłodowska University, pl. Marii Curie-Skłodowskiej 1,  
20-031 Lublin, Poland*

The discovery of graphene started a new branch of material science, one that is oriented towards two-dimensional structures. In the last two decades much focus has been pointed towards materials such as 2D-Xenes or transition metal dichalcogenides – focus based on their unique properties. One interesting example is silicene – silicon analogue of graphene, with high potential compatibility with modern silicon technology [1].

As silicene is volatile in free-standing form, it requires a support. There are numerous already reported candidates suitable [2], with one especially interesting: Si(111) [3]. By depositing ultrathin metal film on Si(111), it is possible to synthesize silicene through silicon atom diffusion. Resulting heterostructure is prepared for further procedures, such as fine-tuning properties by means of chemical functionalization [4].

The preliminary studies of chemical functionalization of silicene on Au/Si(111) heterostructure will be presented. Such structure will be investigated by means of surface science tools, such as scanning tunneling microscope (STM) or reflection high energy electron diffraction (RHEED), performed in-situ in ultra-high vacuum (UHV) conditions. Results reveal the chemophysical properties of silicene and establish a basis of future, application-oriented studies.

### References

- [1] L. Tao et al., *Nature Nano.* 10 (2015), 227
- [2] M. Krawiec, *J. Phys.: Condens. Matter* 30 (2018), 233003
- [3] T. Jaroch et al., *2D Mater.* 8 (2021), 0350380
- [4] M. Kopciuszynski et al., *Scripta Materialia* 252 (2024), 116263

### Acknowledgments

We acknowledge financial support from the National Science Centre of Poland through the OPUS project no. 2022/45/B/ST5/01018

## Possible strain-induced Mott transition in graphene and nanoscale Aharonov-Bohm effect in carbon nanotubes

A. Rycerz<sup>1</sup>, G. Rut<sup>2</sup>, M. Fidrysiak<sup>1</sup>, and D. Goc-Jagło<sup>1</sup>

<sup>1</sup>*Institute of Theoretical Physics, Jagiellonian University, Łojasiewicza 11, PL-30348, Kraków, Poland*

<sup>2</sup>*Verisk Analytics Sp. z o.o., Rakowicka 7, PL-31511 Kraków, Poland*

In two-dimensional crystals, such as graphene, atomic bond lengths can be modified by more than 10 percent by applying in-plane strain, which may lead to significant changes in the electronic structure of the system. We find, by using computationally inexpensive techniques, including the Gutzwiller Wave Function (GWF) and different variants of Gutzwiller Approximation (GA), that uniaxial strain in the armchair direction of graphene layer lead to a significant reduction in the critical Hubbard repulsion ( $U_c$ ) separating the semimetallic phase from the antiferromagnetic Mott insulator. Although graphene stays in the semimetallic phase even for extremely high uniaxial strains, it is predicted to show some measurable signatures of electron correlations, such as the band narrowing and the reduction in double occupancies. The situation is modified in a nanotube geometry, for which uniaxial strain induces approximately periodic gap oscillations, which can be regarded as a nanoscale version of the Aharonov-Bohm effect for strain-induced vector potential. In particular, for small semiconducting nanotube with zigzag edges and realistic value of the Hubbard repulsion ( $U/t_0 = 1.6$ , with  $t_0 \approx 2.5$  eV being the equilibrium hopping integral) energy gap can be reduced by a factor of more than 100 due to the strain. As a result, the system is predicted to show (at the half-filling) strain-induced transition from a nanoscale band insulator to a narrow-gap nanoscale Mott insulator, and *vice-versa*.

### References

- [1] G. Rut, M. Fidrysiak, D. Goc-Jagło, and A. Rycerz, *Int. J. Mol. Sci.* **24**, 1509 (2023). <https://doi.org/10.3390/ijms24021509>.  
[2] A. Rycerz, M. Fidrysiak, D. Goc-Jagło, *J. Magn. Magn. Mater.* **587**, 171322 (2023). <https://doi.org/10.1016/j.jmmm.2023.171322>.

### Acknowledgments

We thank Józef Spałek for discussions. Support from the National Science Centre of Poland (NCN), via Grant No. 2014/14/E/ST3/00256, at the early stage is acknowledged. Computations were partly performed using the PL-Grid infrastructure.

## Temperature influence on direct and indirect bandgap transitions in aluminum alloyed boron nitride

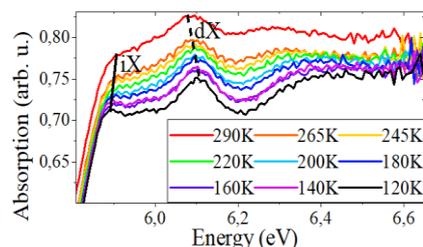
L. Miler, J. Iwański, A. K. Dąbrowska, M. Tokarczyk, J. Binder  
and A. Wysmołek

*Faculty of Physics, University of Warsaw, Pasteura 5, 02-093 Warsaw, Poland*

Ultraviolet light in range between 200 and 280 nm (UV-C) shows excellent germicidal properties. It makes it very useful for sterilization of air, water, surfaces in research laboratories or medical and hospital settings as well as for disinfection in wastewater treatment or even various stages of food and beverage industrial processes [1]. However, UV-C sources being currently in use are mostly based on a mercury vapour, which is highly toxic. Thus, it is crucial to find a safe material that could substitute mercury. A great solution could be to use semiconductor light source, however light emission efficiency dramatically drops with decreasing wavelength leading to efficiency as low as 1% in UV-C spectral range [2]. To overcome this problem application of a novel semiconductor material is needed. We propose to use two-dimensional hexagonal boron nitride, as this compound exhibits intense luminescence in the UV-C surpassing aluminum nitride which is commonly used in this spectral region [2-3]. Alloying boron nitride with aluminum allows the manipulation of material's optical bandgap [4], thus the emission wavelength could be optimized for the desired applications covering the whole UV-C range.

In this communication we studied optical absorption spectra of set of epitaxial boron aluminum nitride samples grown on 2-inch sapphire substrates by Metal-Organic Vapor Phase Epitaxy (MOVPE) with different aluminum concentration. We have found that for alumina alloyed layers new excitonic structure appears at the energy, which coincides with the energy of hBN indirect bandgap transition [5], which is presented in Fig. 1. In order to confirm the indirect character of this transition we performed temperature dependent measurements (10-300 K) of the excitonic absorption lines. We observed that the absorption peaks assigned to direct and indirect excitonic transition are characterized by different temperature behaviour. The obtained results are discussed in terms of the modifications of conduction band electronic structure induced by Al incorporations.

Acknowledgments: This work has been partially supported by the National Science Centre, Poland, under decisions 2022/47/B/ST5/03314 and 2022/45/N/ST5/03396.



**Figure 1.** Absorption spectra of BAlN epitaxial layers measured at different temperatures (120-290 K). Dashed and solid lines indicate the energy of direct and indirect bandgap transitions in hBN, respectively.

### References

- [1] T. Nicolau et al. *Materials*, 15(8), 2854 (2022)
- [2] H. Amano et al. *J. of Phys. D: Appl. Phys.* 1361-6463 (2020)
- [3] A. Maity, et al., *Prog. Quantum. Electron.*, 76(100302), 100302 (2021)
- [4] Q. Zhang et al. *Appl. Surf. Sc.* 0169-4332 (2022)
- [5] J. Iwański et al. <https://arxiv.org/abs/2305.15810> (2023)

## Transport properties of a topological insulator sandwiched between ferromagnetic layers

P. Pigoń<sup>1</sup> and A. Dyrdał<sup>2</sup>

<sup>1</sup>AGH University of Krakow, al. Mickiewicza 30, 30-058 Kraków, Poland

<sup>2</sup>Adam Mickiewicz University in Poznań, ul. Wieniawskiego 1, 61-712 Poznań, Poland

Topological insulators and topological phase transitions have received enormous attention, mainly due to their potential applications in spintronics, next-generation electronics, and quantum information. The dissipationless surface/edge states of topological insulators provide challenges for new generation low-power-consuming electronic devices. In turn, strong spin-orbit interaction in these materials makes them an excellent platform for spin-charge conversion protocols, mainly via current-induced spin polarization.

We will present results of our recent study on thin film 3D topological insulators sandwiched between ferromagnetic layers [1-3]. The hybridization of the top and bottom surface states opens an energy gap in the spectrum of surface states, and magnetic proximity effects (due to adjacent ferromagnetic layers) allow for its further modification. Moreover, the time-reversal symmetry breaking in such a system allows for the observation of anomalous Hall effect and topological phase transition from trivial to Chern or axion insulator phase. Using Green function formalism and linear response theory (Kubo formalism), we derived the anomalous Hall effect (AHE) conductivity and current-induced spin polarization (CISP) in such a hybrid structure. We will present a detailed analysis of the AHE and CISP in the presence and absence (thick films) of hybridization, under external gate voltage, and for various configurations of magnetizations in adjacent ferromagnetic layers.

### References

- [1] P. Pigoń, A. Dyrdał, J. Magn. Magn. Mater. 591 (2024) 171795.
- [2] P. Pigoń, A. Dyrdał, to be published
- [3] A. G. Moghaddam, A. Qaiumzadeh, A. Dyrdał, J. Berakdar, Phys. Rev. Lett 125 (2020) 196801.

### Acknowledgments

This work has been supported by the National Science Centre in Poland under the project Sonata-14 no. 2018/31/D/ST3/023510.

## Magnetotransport in nonstoichiometric and Mn-doped Bi<sub>2</sub>Te<sub>3</sub> 2D flakes

M. Chrobak<sup>1,2</sup>, A. Trembułowicz<sup>2</sup>, A. Naumov<sup>2</sup>, and  
M. Przybylski<sup>1,2</sup>

<sup>1</sup>*Faculty of Physics and Applied Computer Science,*  
<sup>2</sup>*Academic Centre for Materials and Nanotechnology,*  
*AGH University of Krakow, Krakow, Poland*

3D topological insulators (TIs), such as bismuth telluride (Bi<sub>2</sub>Te<sub>3</sub>), can be characterized as materials of an insulating/semiconducting volume and topologically protected conductive surface states. The surface states form a characteristic spin-momentum-locked Dirac cone due to the linear dispersion relation. Such an electronic structure makes TIs a very promising candidate both for research on their unique phenomena related to this non-trivial topology and for potential applications. However, due to structural defects in a real sample, the Fermi level ( $E_F$ ) located in the gap for the volume states is difficult to be achieved [1, 2]. Thus, a control over their electronic structure is important to satisfy the theoretical predictions and increase the scope of technological applicability. 2D films or exfoliated flakes of TIs feature topologically protected conductive one-dimensional boundaries, which allow electrons to travel only in two paths. Moreover, as a consequence of spin-momentum locking, all the electrons traveling in one direction are spin up and all the electrons traveling in the opposite direction are spin down. Doping a TI with magnetic ions breaks the time reversal symmetry, allowing one direction to exist without the other one. Such behaviour, called the quantum anomalous hall effect (QAHE) [3], opens new possible applications like a precisely known resistance at a zero magnetic field, which was not possible in the case of the standard quantum Hall effect.

In the presence of a magnetic field Landau quantization of energy levels appears [4]. Since only carriers with energies close to  $E_F$  participate in transport, a rapid increase in the density of states by the Landau level causes a rapid increase in conductivity. In this way, as the Landau levels passes through the  $E_F$ , oscillations in resistance as a function of the magnetic field, known as Shubnikov–de Haas (SdH) quantum oscillations, may be observed.

In this contribution, we compare the electronic structure of Bi<sub>2-x</sub>Te<sub>3+x</sub> probed by SdH oscillations, for x up to 0.14, with that detected locally by scanning tunnelling spectroscopy and calculated by DFT. Moreover we discuss the results of magnetoresistance and Hall effect measurements at sub-Kelvin temperatures for an Mn-doped Bi<sub>2</sub>Te<sub>3</sub> TI for both as-grown single crystals and 2D flakes. The flakes were obtained by exfoliation with the help of an adhesive tape performed until the desired flake thickness was achieved. The results for a ~30 nm thick flake have shown that exfoliation does not affect the magnetic properties of the flake and a fractional QAHE has been observed.

### References

- [1] M Chrobak et al., J. Magn. Magn. Mater. **589**, (2024) 171548.
- [2] K. Nowak et al., Materials **15**, (2022) 2083.
- [3] X. Kou et al., Nature Communications **6**, (2015) 8474.
- [4] M. Chrobak et al., New Journal of Physics **22**, (2020) 063020.

### Acknowledgments

Project supported by the program “Excellence initiative research university” for the AGH University of Krakow

## Computational analysis of two-dimensional alloy based systems

M. Szyszko<sup>1</sup>, M. E. Marchwiany<sup>2</sup>, T. Woźniak<sup>1</sup> and M. Birowska<sup>1</sup>

<sup>1</sup> *University of Warsaw, Faculty of Physics, 00-092 Warsaw, Pasteura 5, Poland*

<sup>2</sup> *Interdisciplinary Centre for Mathematical and Computational Modelling (ICM),  
University of Warsaw, Pawińskiego 5a, 02-106 Warsaw, Poland*

Transition metal dichalcogenides (TMDs) are emerging as highly versatile materials due to their unique properties. These two-dimensional van der Waals (vdW) materials have shown immense potential in various applications [1, 2], including nanoelectronics, spintronics and catalysis, owing to their direct band gaps, strong spin-orbit coupling and mechanical properties. Doping these materials with other elements is the next step towards fine-tuning their properties to specific uses [3]. The understanding of the correlation between the distribution of the dopants within the host and various properties of desired nanomaterials plays a crucial role in designing nanomaterials with particular functionality.

Our work is twofold, we consider both ordered and disordered alloys based on ab initio and Monte Carlo approaches, respectively. In the first part, we generate a workflow for computing various properties of the alloys within the accuracy of the DFT method. We perform high throughput computations for all non-equivalent positions of dopants in desired supercell size, and we reduce the configuration space by applying the symmetry operations. We consider sizes of the supercell accessible within the DFT calculations on massively parallel supercomputers. As an example we present results for  $\text{Mo}_{1-x}\text{W}_x\text{S}_2$  systems up to a cell of 4x4 size. Next, by using the Monte Carlo method, we identify energetically favorable configurations in large systems, focusing on whether the dopants form clusters or are uniformly distributed. Following the structural analysis, we will examine the electronic properties of the generated systems. Based on these results, the extensive computational data produced will be compiled into a robust database, which will subsequently be utilized in machine learning algorithms. The aim of these algorithms is to predict novel applications and the properties of TMD alloys based on their composition. This approach also facilitates the engineering of materials tailored to specific desired properties.

### References

- [1] Khan, K.; Tareen, A.K.; Aslam, M.; Wang, R.; Zhang, Y.; Mahmood, A.; Ouyang, Z.; Zhang, H.; Guo, Z. *J. Mater. Chem. C* 2020, 8, 387–440.
- [2] Bao, Q.; Hoh, H.Y.; Elsevier: Amsterdam, The Netherlands, 2020; p. 326.
- [3] A. Harchol, S. Zuri, E. Ritov, F. Horani, M. M. Rybak, T. Wozniak, A. Eyal, Y. Amouyal, M. Birowska and E. Lifshitz, 2024 *2D Mater.* 11 035010

## Effect of Fe-doping on VS<sub>2</sub> monolayer: A first-principles study

M. Jafari<sup>1</sup>, N. Rahmani<sup>2</sup> and A. Dyrdał<sup>1</sup>

<sup>1</sup>*Faculty of Physics, ISQI, Adam Mickiewicz University in Poznań, ul. Uniwersytetu  
Poznanskiego 2, 61-614 Poznań, Poland*

<sup>2</sup>*Materials Simulation Laboratory, Department of Physics, Iran University of Science and  
Technology, Tehran 1684613114, Iran*

Using the ab-initio approach based on the Density Functional Theory (DFT), we have investigated the effects of iron (Fe) doping on the properties of vanadium disulfide (VS<sub>2</sub>) monolayer [1]. The Transition Metal Dichalcogenides (TMDs), especially VS<sub>2</sub>, are of great interest due to their electronic, magnetic, and optical properties, that make these materials very promising for applications in novel spintronics, electronics, and biomedical sciences. In contrast to most TMD materials, which are typically non-magnetic, pure VS<sub>2</sub> exhibits intrinsic ferromagnetism. In addition, one can enhance the electronic and magnetic properties of VS<sub>2</sub> by doping it with Fe atoms [2].

Our results show a strong modification of the electronic and magnetic properties of VS<sub>2</sub> monolayer by the presence of Fe atoms. First, the Fe atoms induce significant magnetic moments in the system [3]. Second, the Fe-doped monolayer of VS<sub>2</sub> reveals the possibility of tuning the energy band gap by a change in concentration and/or location of the dopants. Our results are in close agreement with the experimental data, which confirm the decrease of bandgap in the VS<sub>2</sub> monolayer with the Fe-doping [4]. We also discuss the applications of the Fe-doped VS<sub>2</sub> in spintronics, optoelectronics, and catalysis. This ability to tune the electronic, magnetic, and optical properties of VS<sub>2</sub> by the Fe doping, extends its applicability not only to electronic and spintronic devices but also to biomedicine (e.g., in cancer therapy). Our work covers both a deep understanding of dopant-induced magnetism in VS<sub>2</sub> monolayer and also provides the way for the novel developments of advanced nanodevices and nanotechnologies.

### References

- [1] Mirali Jafari, Nasim Rahmani and Anna Dyrdał, to be published
- [2] M. Kan, B. Wang, Y. H. Lee, and Q. Sun, Nano Research 8, 1348 (2015).
- [3] A. K. Yadav, C. Patel, G. Kiran, R. Singh, A. K. Singh, V. Garg, S. Mukherjee, and S. K. Pandey, The European Physical Journal B 96, 49 (2023).
- [4] H. Lei, X. Wang, S. Bai, F. Gong, N. Yang, Y. Gong, L. Hou, M. Cao, Z. Liu, and L. Cheng, ACS Applied Materials & Interfaces 12, 52370 (2020).

### Acknowledgments

This work has been supported by the Norwegian Financial Mechanism under the Polish – Norwegian Research Project NCN GRIEG “2Dtronics” no. 2019/34/H/ST3/00515.

## Using image-potential states as local probes for magnetic Gr-hybrid systems

A. Schlenhoff

*Institute of Physics, University of Münster, Germany*

Image-potential states (IPSs) evolving in front of polarizable surfaces are known to serve as quantum sensors for various properties ranging from electron reflectivity of surfaces over surface magnetization to interfacial coupling at buried interfaces [1,2]. They can be locally studied by means of resonant scanning tunnelling microscopy (STM) and spectroscopy (STS), and their study has been applied to metals, metal surfaces with nanostructures, semiconductors, insulators, topological and 2D materials. Particularly, analysis of IPSs have found wide application to map surface work function changes [3] and by this means have been proposed for mapping shifts of the Dirac point in respective materials [4]. Recently, IPSs have also been demonstrated to be sensitive to atomic-scale surface spin textures of metallic thin-films on heavy element substrates, as revealed by spin-polarized STM and STS [5], allowing to map non-collinear magnetic surfaces with atomic resolution but at nanometer distances [6].

In this talk, I will present spin- and laterally-resolved STM and STS studies of IPSs on iron (Fe)-intercalated graphene (Gr) on an Ir(111) substrate. Fe is known to grow pseudomorphically on the Ir substrate, while the Gr overlayer exhibits a strong buckling within the moiré unit cell, resulting in a laterally varying hybridization to the metal and thus a laterally varying spin-polarization [7]. Our studies reveal that, due to the sensitivity of the IPSs to the interlayer coupling of Gr to the ferromagnetic substrate and its resulting spin-polarization, the IPSs exhibit an energy- and position-dependent spin-polarization within the moiré unit cell, allowing to use these states as local probes of the graphene magnetism [8]. The moiré of Gr/Fe/Ir(111) is characterized by three high symmetry regions where the middle of the carbon ring is located either on-top, in a fcc or hcp position over the substrate atom. For this system, however, conventional STM only shows a strong contrast between the top area and the entire rest which is then collectively called “valley” [7]. Interestingly, we find that the IPSs are strongly affected by the different stackings within the moiré unit cell providing a distinctive contrast between the fcc and hcp regions in topography images and  $dI/dU$  maps recorded in the resonant tunneling mode [8]. Consequently, our spin- and laterally-resolved STM and STS studies demonstrate, that resonant tunneling through IPSs allows for the simultaneous imaging of morphology and spin texture within the moiré unit cell, even providing access to surface properties that remain hidden in conventional STM. We therefore see great potential in applying this technique to other 2D materials such as twisted van der Waals materials or 2D magnetic semiconductors.

### References

- [1] D. Niesner and Th. Fauster, *J. Phys.: Condens. Matter* 26 (2014) 393001.
- [2] S. Bose *et al.*, *New J. Phys.* 12 (2010) 023028.
- [3] A. Schlenhoff *et al.*, *Appl. Phys. Lett.* 120 (2022) 261601.
- [4] F. Craes *et al.*, *Phys. Rev. Lett.* 111, (2013) 056804.
- [5] A. Schlenhoff *et al.*, *Phys. Rev. Lett.* 123 (2019) 037201.
- [6] A. Schlenhoff *et al.*, *Appl. Phys. Lett.* 116, (2020) 122406.
- [7] R. Decker *et al.*, *J. Phys.: Condens. Matter* 26 (2014) 394004.
- [8] M. Bazarnik *et al.*, in preparation.

## Heat transport in quantum materials with a cool twist

K.-J. Tielrooij<sup>1,2</sup>

<sup>1</sup>*Catalan Institute of Nanoscience and Nanotechnology (ICN2), BIST & CSIC, Campus UAB, 08193 Bellaterra (Barcelona), Spain*

<sup>2</sup>*Eindhoven University of Technology, Den Dolech 2, 5612 AZ, Eindhoven, the Netherlands*

Quantum materials exhibit several exciting ultrafast physical phenomena that are moreover potentially technologically useful. This is particularly true for quantum materials with massless Dirac electrons, such as graphene and topological insulators. When light is absorbed in these materials, electron heating occurs through electron-electron interactions on a 10-100 fs timescale, followed by electron cooling, typically involving the emission of phonons on a picosecond timescale.

Whereas these ultrafast thermodynamics in monolayer graphene are relatively well understood, this is not the case for twisted bilayer graphene near the magic angle. Using time-resolved photocurrent measurements, we have studied these dynamics and found that the electron cooling dynamics in twisted bilayer graphene near the magic angle is very distinct from the dynamics in monolayer or non-twisted bilayer graphene. Specifically, the cooling time in near-magic twisted bilayer graphene is a few picoseconds all the way from room temperature down to 10 K. We ascribe these observations to Umklapp-assisted electron-phonon cooling, facilitated by the moiré pattern in twisted bilayer graphene [1]. Whereas Umklapp scattering is a very common phenomenon for phonons, it is very rare to observe such scattering processes for electrons. These results establish twist angle as control knob for steering the cooling dynamics and flow of electronic heat, and have possible implications for the development of ultrafast detectors operating at cryogenic temperatures, among others.

We have also exploited the ultrafast thermodynamics in quantum materials to generate harmonics in the terahertz (THz) regime [2], which is particularly efficient in “quantum metamaterials” consisting of a quantum material and a metallic grating [3]. Thanks to an efficient “Coulomb cooling” mechanism between surface and bulk electronic states in topological insulators [4], we have recently demonstrated that the ultrafast thermodynamics can give rise to third-order terahertz harmonic generation approaching the milliwatt regime [5]. Furthermore, quantum metamaterials enable fast and gate-tunable conversion from THz light to visible light [6]. These results establish quantum materials as an excellent material platform for nonlinear terahertz photonics, with possible applications in next-generation wireless communication systems, among others.

### References

- [1] J. Mehew *et al.*, *Sci. Adv.* 10 (2024) eadj1361.
- [2] H.A. Hafez *et al.*, *Nature* 561 (2018) 507.
- [3] J.C. Deinert *et al.*, *ACS Nano* 15 (2021) 1145.
- [4] A. Principi and K.J. Tielrooij, *Phys. Rev. B.* 106 (2022) 115422.
- [5] K.J. Tielrooij *et al.*, *Light: Sci. Appl.* 11 (2022) 315.
- [6] I. Ilyakov *et al.*, *Nano Lett.* 23 (2023) 3872.

## Magnetolectric fractals, magnetolectric parametric resonance and Hopf bifurcation

M. Wanic<sup>1</sup>, Z. Toklikishvili<sup>2</sup>, S. K. Mishra<sup>3</sup> M. Trybus<sup>1</sup> and L. Chotorlishvili<sup>1</sup>

<sup>1</sup>*Department of Physics and Medical Engineering, Rzeszów University of Technology, 35-959 Rzeszów, Poland*

<sup>2</sup>*Faculty of Exact and Natural Sciences, Tbilisi State University, Chavchavadze av.3, 0128 Tbilisi, Georgia*

<sup>3</sup>*Department of Physics, Indian Institute of Technology (Banaras Hindu University), Varanasi 221005, India*

In the present work, we study the dynamics of the magnetic nanodisc coupled through a magnetolectric coupling to a ferroelectric crystal. The model of our interest is nonlinear, and we explore the problem under different limits of weak and strong non-linearity. By applying two electric fields with different frequencies, we control the form of the confinement potential of a ferroelectric subsystem and realize different types of dynamics. We proved that the system is more sensitive to magnetolectric coupling in the case of double-well potential. In particular, in the case of strong non-linearity, arbitrary small values of magnetolectric coupling lead to chaotic dynamics. In essence, magnetolectric coupling plays a role akin to the small perturbations destroying invariant tori according to the KAM theorem. We showed that bifurcations in the system are of Hopf's type. We observed the formation of magnetolectric fractals in the system. In the limit of weak non-linearity, we studied a problem of parametric nonlinear resonance and enhancement of magnetic oscillations through magnetolectric coupling.

### References

[1] M. Wanic<sup>1</sup>, Z. Toklikishvili<sup>2</sup>, S. K. Mishra<sup>3</sup> M. Trybus<sup>1</sup>, L. Chotorlishvili<sup>1</sup> *Physica D* 467, 134257 (2024).

## Spin mixing parameter as an indicator of Ising type-II pairing

P. Jureczko<sup>1</sup>, J. Haniš<sup>2</sup>, P. E. Faria Junior<sup>3</sup>, M. Gmitra<sup>2,4</sup> and M. Kurpas<sup>1</sup>

<sup>1</sup>*Institute of Physics, University of Silesia in Katowice, 41-500 Chorzów, Poland*

<sup>2</sup>*Institute of Physics, Pavol Jozef Šafárik University in Košice, Park Angelinum 9, 04001 Košice, Slovakia*

<sup>3</sup>*Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany*

<sup>4</sup>*Institute of Experimental Physics, Slovak Academy of Sciences, Watsonova 47, 04001 Košice, Slovakia*

We present an efficient, fully ab initio approach to determine possible Ising type-II pairing [1] in centrosymmetric superconductors based on the spin mixing parameter  $b^2$ .

We show [2], that the spin polarization of degenerate Bloch bands and the direction of intrinsic spin-orbit (Zeeman) fields being essential to the Ising pairing can be associated with the parameter  $b^2$ . Using first-principles calculations we calculate  $b^2$  for individual Fermi pockets of monolayer transition metal dichalcogenide superconductors PdTe<sub>2</sub>, NbTe<sub>2</sub>, and TiSe<sub>2</sub> with the 1T structure, and provide a general picture of possible Ising type-II pairing within the full Brillouin zone. To complement our first-principles results, we use group theory to provide a detailed picture of spin-orbit coupling and spin mixing in the relevant bands forming Fermi pockets. Finally, by connecting the spin-mixing parameter  $b^2$  with the intrinsic out-of-plane Zeeman field, we estimate the upper in-plane critical magnetic field.

The proposed method is very versatile and its application is not restricted only to 2D systems. It can be used to extend high-throughput screening calculations of 2D Ising type-II superconductors [3] and can give an insight into SOC contribution to the critical field anisotropy in bulk superconductors.

### References

- [1] M. Liao, et al., Nat. Phys. 14, (2018) 344.
- [2] P. Jureczko, J. Haniš, P. E. Faria Junior, M. Gmitra, and M. Kurpas, Phys. Rev. B 109, (2024) 165428
- [3] C. Wang, B. Lian, X. Guo, J. Mao, Z. Zhang, D. Zhang, B.-L. Gu, Y. Xu, and W. Duan, Phys. Rev. Lett. 123, (2019) 126402.

### Acknowledgments

PJ. and M.K. acknowledge support from the Interdisciplinary Centre for Mathematical and Computational Modelling (ICM), University of Warsaw (UW), within grant no. G83-27. The project is financed by the National Center for Research and Development (NCBR) under the V4-Japan project BGapEng V4-JAPAN/2/46/BGapEng/2022.

## Ultrafast dynamics of excitons in monolayers of semiconductor TMDs

P. Kossacki

*Faculty of Physics, University of Warsaw, ul. Pasteura 5, 02-093 Warsaw, Poland*

Monolayers of transition metal dichalcogenides (TMDs) draw a lot of attention as semiconducting materials with robust optical properties, strong Coulomb interaction and an optically accessible valley degree of freedom. Extraordinary properties of exciton complexes lead to new possibilities of exploration of nonlinear effects.

In my talk, I will focus on ultrafast studies of exciton dynamics explored by time resolved photoluminescence, FWM and femtosecond pump-probe experiments. The studies of neutral and charged exciton optical response show strong interactions between different complexes. For example creation of CX population in a given K,K' valley leads to the capture of available free carriers in the opposite valley and reduces the interaction of neutral X with the Fermi sea. From the valley-resolved analysis of the observed effects we are also able to extract the spin-valley relaxation times of free carriers as a function of carrier density. The several effects related to interaction with carries such as the oscillator strength variation and energy shift will be discussed and compared to the cases of ordinary quantum wells. I will point similarities and differences in the complex landscape of exciton-exciton and exciton-carrier interactions in both two dimensional systems.

### References

- [1] Aleksander Rodek et al. 2023 2D Materials 10, 025027,
- [2] Kacper Oreszczuk et al. 2023 2D Materials 10, 045019.

## Optomechanics of time-varying plasmonic-semiconducting nanomembranes

A. K. Dhiman,<sup>1</sup> K. Sympoura<sup>1,2</sup>, T. Vasileiadis<sup>1</sup> and B. Graczykowski<sup>1</sup>

<sup>1</sup>*Faculty of Physics, Adam Mickiewicz University, Uniwersytetu Poznańskiego 2, 61-614  
Poznan, Poland*

<sup>2</sup>*Department of Physics, University of Patras, Patras, Greece.*

When light is impinged on a surface, it deposits momentum that can initiate mechanical motions. This “opto-mechanical” coupling can be exploited in signal-processing devices to convert microwave radiation into more manageable acoustic phonons for timing and frequency filtering operations [1]. Moreover, data centers can use optomechanics to encode gigahertz (GHz) signals into light that travels via optical fibers. Some very promising nanomaterials for these developments are plasmonic-semiconducting nanomembranes. The semiconductor can offer strong photoelastic coupling, while the plasmonic metal can harvest electromagnetic energy. The two-dimensional (2D) morphology can lead to higher operational frequencies through spatial confinement of GHz phonons.

In this talk, we will present an additional reason for considering 2D heterostructures as promising materials for future signal-processing applications. That is the ability to control their optical, electronic, and mechanical properties at ultrafast timescales using femtosecond laser pulses [2]. Our work is based on a recently developed experimental technique termed pump-Brillouin light scattering [3] (pump-BLS), as well as detailed theoretical modeling of carrier-phonon-photon interactions. Finally, we will explain why transition metal dichalcogenides are promising materials for applications requiring strong photoelasticity [4] and ultrafast charge transfer [5].

### References

- [1] T. Vasileiadis *et al.*, *Journal of Applied Physics*, 2021, 129(16), 160901.
- [2] R. Białek *et al.*, *Photoacoustics*, 2023, 30, 100478.
- [3] T. Vasileiadis *et al.*, *Science Advances*, 2020, 6(51), eabd4540.
- [4] V. Babacic *et al.*, *Advanced Materials*, 2021, 33(23), 2008614.
- [5] T. Pincelli *et al.*, *Advanced Materials*, 2023, 35(9), 2209100.

### Acknowledgments

This project was supported by the National Science Center of Poland (NCN) with the Sonata Grant No. 2021/43/D/ST3/02526, as well as UMO-2018/31/D/ST3/03882. We are thankful to our collaborators, Mikołaj Pochylski, Jacek Gapinski, Piotr Graczyk, and Rafal Bialek, who are part of the ongoing work.

## Raman optical activity of the charge density wave-related phonon modes in 2H-TaSe<sub>2</sub> – a study by Raman scattering

J. Kossacki<sup>1</sup>, I. Lutsyk<sup>2</sup>, P. Kowalczyk<sup>2</sup>, N. Zawadzka<sup>1</sup>, J. Binder<sup>1</sup>, M. R. Molas<sup>1</sup>  
and A. Wysmolek<sup>1</sup>

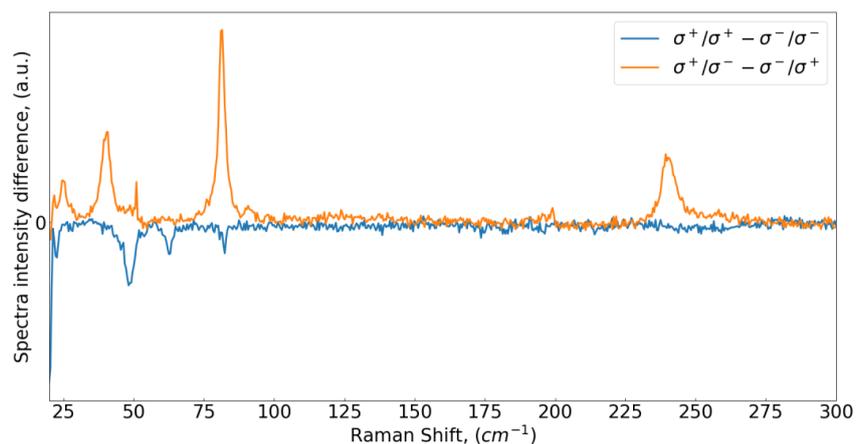
<sup>1</sup>*Institute of Experimental Physics, Faculty of Physics, University of Warsaw, Warsaw, Poland*

<sup>2</sup>*Faculty of Physics and Applied Informatics, University of Lodz, Lodz, Poland*

Transition metal dichalcogenides have many interesting properties and have been an object of investigation for many years [1]. One of such intriguing properties are charge density waves (CDWs), a periodic lattice distortion present at low temperatures in some of the TMDs, such as 1T-TaS<sub>2</sub> and 1T-TiSe<sub>2</sub>.

The object of this study, the 2H polytype of TaSe<sub>2</sub> develops different kinds of CDWs below 120K. As the unit cell grows, new phonon modes emerge, which renders the Raman scattering especially attractive for investigating the nature of these CDWs. Moreover, recent investigation [2] shows that CDW states can show interesting chiral properties, which give rise to Raman optical activity (ROA), a property especially attractive for potential use in spintronics and data storage.

The symmetries of the CDW-related phonon modes were investigated with the aid of Raman scattering. Figure 1 shows the differences between the Raman spectra measured in different configurations of circular polarizations of excitation and detection. ROA phenomenon is observed, and a correlation between phonon symmetry and their chiral properties can be traced. These results will be discussed in the context of the material band structure and the general properties of the CDW phases.



**Figure 1.** Differences between Raman spectra measured in different configurations of circular polarizations of excitation/detection

### References

- [1] Q. Wang *et al.*, Nature Nanotech **7**, (2012) 699–712  
[2] E. M. Lacinska *et al.*, Nano Lett. **22**, 7 (2022) 2835-2842

## GRANAD – framework and code for optoelectronic properties of low-dimensional structures

M. Pelc<sup>1</sup>, D. Dams<sup>2</sup>, M. Kosik<sup>1</sup>, M. Muller<sup>2</sup>, A. Ghosh<sup>1</sup>, J. Szczuczko<sup>1</sup>, G. W. Bryant<sup>3</sup>, A. Ayuela<sup>4</sup>, C. Rockstuhl<sup>2,5</sup> and K. Słowik<sup>1</sup>

<sup>1</sup>*Institute of Physics, Nicolaus Copernicus University in Toruń, Grudziądzka 5/7, 87-100 Toruń, Poland*

<sup>2</sup>*Karlsruhe Institute of Technology, Institute of Theoretical Solid State Physics, Kaiserstr. 12, 76131 Karlsruhe, Germany*

<sup>3</sup>*Joint Quantum Institute, University of Maryland and National Institute of Standards and Technology, College Park 20742, MD, USA; Nanoscale Device Characterization Division, National Institute of Standards and Technology, Gaithersburg 20899, MD, USA*

<sup>4</sup>*Centro de Fisica de Materiales, CFM-MPC CSIC-UPV/EHU, Paseo Manuel Lardizabal 5, Donostia-San Sebastian 20018, Spain; Donostia International Physics Center (DIPC), Paseo Manuel Lardizabal 4, Donostia-San Sebastian 20018, Spain*

<sup>5</sup>*Karlsruhe Institute of Technology, Institute of Nanotechnology, Kaiserstr. 12, 76131 Karlsruhe, Germany*

Low-dimensional structures like 1D atomic chains and 2D nanoflakes have unique electronic, optical, and material properties due to their chemical composition and geometry. They can be used as elementary building blocks in heterostructures realizing nanoscaled optoelectronics tuned by electronic or optical means or in the presence of atomic defects (adatoms) [1]. In reverse, a flake or chain can be exploited to modulate the dynamics of adatoms positioned in its vicinity [2].

We have developed a theoretical framework and a related python toolbox, GRANAD (Graphene Nanoantennas with ADatoms) [3], to study these properties. The framework combines a tight-binding approach to model the electronic properties of 2D nanoflakes with the master equation approach to capture electron dynamics. The single-electron model allows for a favorable linear scaling of the Hilbert space size with the number of carbon sites, allowing us to study relatively large flakes. Originally developed to model graphene, the code has recently been extended to include different 2D materials and their stacks.

I am going to present the capabilities of the GRANAD toolbox and the selected results we have obtained. In particular, the framework has been recently applied to investigate the nature of plasmonic excitations on graphene nanoflakes [4] or the influence of atomic defects on the optical properties of low-dimensional material structures [1, 2].

### References

- [1] M. M. Müller, M. Kosik, M. Pelc, G. W. Bryant, A. Ayuela, C. Rockstuhl, K. Słowik, *Phys. Rev. B* 104, 235414 (2021).
- [2] M. Kosik, M. M. Müller, K. Słowik, G. W. Bryant, A. Ayuela, C. Rockstuhl, M. Pelc, *Nanophotonics*, 11, 3281-3298 (2022).
- [3] D. Dams, M. Kosik, M. Muller, A. Ghosh, J. Szczuczko, G.W. Bryant, A. Ayuela, C. Rockstuhl, M. Pelc, K Słowik, Submitted to *Comp. Phys. Commun.*
- [4] M. M. Müller, M. Kosik, M. Pelc, G. W. Bryant, A. Ayuela, C. Rockstuhl, K. Słowik, *J. Phys. Chem. C* 124, 24331–24343 (2020).

## Raman studies of homoepitaxial hBN grown by MOVPE on isotopically-pure h<sup>10</sup>BN exfoliated flakes - PCA analysis

P. Maksymiuk<sup>1</sup>, A. K. Dąbrowska<sup>1</sup>, P. Tatarczak<sup>1</sup>, R. Bożek<sup>1</sup>, R. Stępniewski<sup>1</sup>, J. Binder<sup>1</sup>, E. Janzen<sup>2</sup>, J. H. Edgar<sup>2</sup> and A. Wysmołek<sup>1</sup>

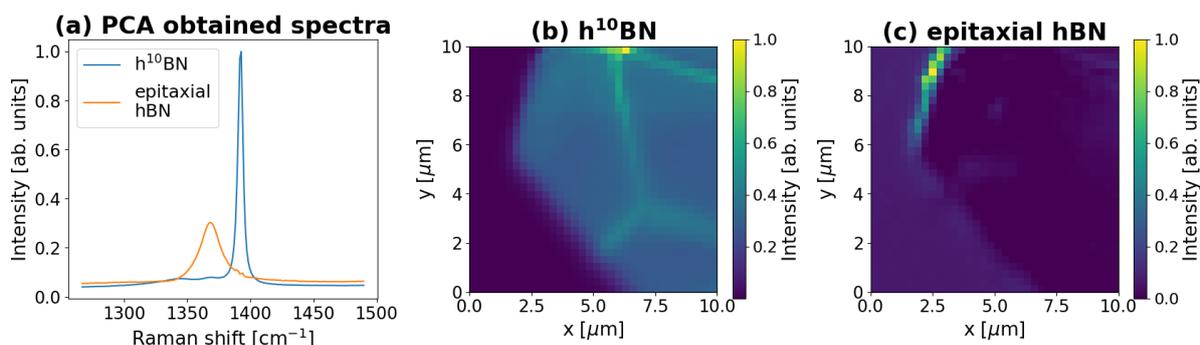
<sup>1</sup> Faculty of Physics, University of Warsaw, Pasteura 5, 02-093 Warsaw, Poland

<sup>2</sup> Tim Taylor Department of Chemical Engineering, Kansas State University, Manhattan, Kansas 66506, USA

Hexagonal boron nitride (hBN) is a two-dimensional semiconductor with a wide bandgap (~ 6 eV) which is a promising material for electronic, optoelectronic, nanophotonic, and quantum sensing devices especially those involving van der Waals structures. The highest structural quality of hBN is typically found in bulk crystals, which must be exfoliated to obtain thin flakes. However, to achieve large-scale layers, epitaxial growth is required. In our laboratory, we utilize Metal-Organic Vapor Phase Epitaxy (MOVPE) to grow epitaxial hBN.

Here we report on the properties of MOVPE hBN grown homoepitaxially on isotopically-pure exfoliated h<sup>10</sup>BN flakes. Raman spectroscopy was employed to obtain spectral data from different regions of the sample and to analyze differences in properties of grown material at different locations on the h<sup>10</sup>BN flakes. Principal component analysis (PCA) of collected Raman spectra showed that epitaxial hBN is present mainly at the edges of h<sup>10</sup>BN flakes (Fig. 1) indicating that the growth starts at the edges or structural defects. This result is consistent with our recent results obtained for homoepitaxial layers grown on hBN flakes exfoliated from crystals with natural isotopic composition [1].

The obtained results open up new possibilities for the development of homoepitaxial growth of hBN and provide a better understanding of the mechanisms determining the properties of the obtained layers.



**Figure 1.** (a) Raman spectra of  $E_{2g}^{\text{high}}$  mode in h<sup>10</sup>BN (blue) and hBN (orange) obtained from PCA, (b) spatial intensity map of the h<sup>10</sup>BN component, (c) spatial intensity map of the hBN component.

### References

[1] J. Binder et al. Nano Letters 24, 6990–6996 (2024)

### Acknowledgments

This work has been partially supported by the National Science Centre, Poland, under decisions 2022/47/B/ST5/03314. hBN crystal growth was supported by the Office of Naval Research, award number N00014-20-1-2474.

## Structural commensurability and incommensurability in twisted van der Waals systems

M. I. Katsnelson

*Institute for Molecules and Materials, Radboud University, Heyendaalseweg 135, 6525AJ, Nijmegen, The Netherlands*

Investigation of Van der Waals heterostructures based on combination of different two-dimensional materials is probably the hottest subfield in the field of two-dimensional materials now. I will discuss basic properties of the most intensively studied heterostructures, twisted bilayer graphene and graphene on hexagonal boron nitride (hBN).

Structural reconstruction due to interplay of interlayer van der Waals and intralayer elastic energies is the key phenomenon in physics of these objects. In particular, it leads to commensurate-incommensurate phase transition at the change of misorientation angle [1]. I will review computational and analytical theoretical approaches to the physics of commensurability and incommensurability and its effect on the electronic structure [2-5]. The metal-insulator transition in graphene on hBN will be also considered within the model of classical critical percolation [6].

Commensurate-incommensurate transition in van der Waals heterostructures can be detected and studied optically, via second-harmonic generation, as was recently predicted theoretically [7] and confirmed experimentally [8].

After this general consideration I will discuss importance of atomic reconstruction in the commensurate phase for the most exciting features of twisted van der Waals systems such as flat band formation.

### References

- [1] C. R. Woods *et al.*, Nature Phys. **10** (2014) 451.
- [2] M. M. van Wijk *et al.*, Phys. Rev. Lett. **113** (2014) 135504.
- [3] G. J. Slotman *et al.*, Phys. Rev. Lett. **115** (2015) 186801.
- [4] M. M. van Wijk *et al.*, 2D Mater. **2** (2015) 034010.
- [5] Yu. N. Gornostyrev and M. I. Katsnelson, Phys. Rev. B **102** (2020) 085428.
- [6] M. Titov and M. I. Katsnelson, Phys. Rev. Lett. **113** (2013) 096801.
- [7] M. Vandelli *et al.*, Phys. Rev. B **99** (2019) 165432.
- [8] E. A. Stepanov *et al.*, ACS Appl. Mater. Interfaces **12** (2020) 27758.

### Acknowledgments

The work is supported by Dutch Research Council (NWO) via the “TOPCORE” consortium.

## Scanning photoelectron spectromicroscopy: from static to operando studies of 1D- and 2D-materials

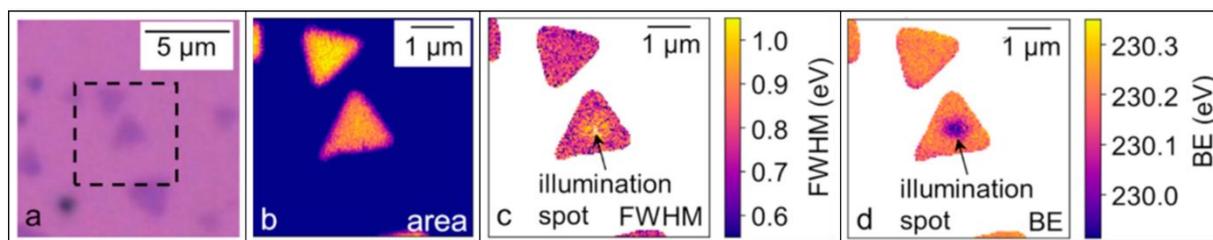
L. Gregoratti, M. Amati and Z. Miłosz

*Elettra Sincrotrone Trieste SCpA – in Area Science Park, Trieste, Italy*

Due to the relatively small size of 1D and 2D materials, like InP nanowires and Graphene or MoS<sub>2</sub> flakes, it is extremely difficult to study their behavior with chemical-sensitive characterization techniques that usually do not offer submicron spatial resolution. In this work, we present the capabilities of photoemission imaging and spectromicroscopy in the chemical and electronic investigation of materials at the submicron scale.

The Scanning PhotoEmission Microscope (SPEM), hosted at the ESCA Microscopy beamline at the Elettra synchrotron light source, uses a direct approach to add the spatial resolution to photoemission and to characterize chemically surfaces at the submicron scale i.e. the use of a small focused X-ray photon probe to illuminate the sample [1]. The focusing of the X-ray beam is performed by using a Zone Plate and the sample surface is mapped by scanning the sample with respect to the focused beam. The X-ray beam can be downsized to a diameter of 130 nm, which allows an imaging resolution of less than 100 nm. The overall energy resolution is better than 200 meV.

Recent achievements in the characterization of 1D and 2D materials will be presented, providing an overview of the capabilities of this powerful technique, for example in the operando surface character-ization of InP Nanowire p–n Junctions [2] or in the investigation of Sulphur vacancy in monolayer MoS<sub>2</sub> [3] (see Figure 1). Moreover the unique capabilities of the SPEM allow also to highlight the effects of the substrate on the properties of low dimensional materials, thanks to the possibility to characterize both free standing, i.e. without any substrate, and supported small samples. In particular, the fine electronic structure as a function of suspended graphene layers [4], will be presented and discussed.



**Figure 1.** Single layer MoS<sub>2</sub> flakes, a) optical image; b) SPEM intensity image at Mo 3d; c) Mo 3d FWHM map; d) Mo 3d BE (eV) map.

### References

- [1] <https://www.elettra.eu/elettra-beamlines/escamicroscopy.html>
- [2] S. R. McKibbin *et al.*, Nano Lett. 20(2) (2020), 887-895.
- [3] T. Grünleitner *et al.*, ACS Nano 16(12) (2022), 20364–20375.
- [4] T. Susi *et al.*, Phys. Rev. Mat., 2, (2018) 074005.

## Investigation of nanoscale electrical properties of epitaxial MoO<sub>3</sub>

A. Nadolska, D. A. Kowalczyk, I. Lutsyk, M. Piskorski, P. Krukowski, P. Dąbrowski, M. Le Ster, W. Kozłowski, R. Dunal, P. Przybysz, W. Ryś, K. Toczek, P. J. Kowalczyk and M. Rogala

*University of Lodz, Department of Solid State Physics, Pomorska 149/153, 90-236 Łódź, Poland*

MoO<sub>3</sub> is a wide bandgap two-dimensional transition metal oxide with high relative permittivity and transparency. Due to these properties, ultrathin layers of molybdenum trioxide are ideal candidates for a wide range of applications, such as in flexible and stretchable electronics, optoelectronics, catalysis, and resistive random access memory.

We performed a nanoscale electrical study of epitaxially grown MoO<sub>3</sub>. The ultrathin layer was deposited under ultrahigh vacuum conditions by thermal evaporation on highly oriented pyrolytic graphite [1-3]. The monolayer, with thickness of 0.7 nm, was examined by X-ray photoelectron spectroscopy, revealing the presence of two components: about 95% is represented by Mo<sup>6+</sup> from the 3d<sub>5/2</sub> component at the 233.2 eV binding energy position and 5% is Mo<sup>5+</sup> 3d<sub>5/2</sub> at 231.8 eV.

Our investigations indicate that the slightly nonstoichiometric MoO<sub>3</sub> monolayers are heterogeneous in terms of electrical conductivity in the nanoscale. The 5+ oxidation state, which is associated with oxygen vacancies in the molybdenum trioxide, locally increases the conductivity. Additionally, an atomic force microscopy (AFM) study showed that MoO<sub>3</sub> islands can be manipulated and moved under slight mechanical stress of the AFM probe. Furthermore, we showed that point stimulation can be used for removal of oxide monolayer with nanoscale precision.

### References

- [1] D. A. Kowalczyk et al., 2D Materials, 8, 025005 (2021)
- [2] D. A. Kowalczyk et al., ACS Appl. Mater. Interfaces, 14, 44506-44515 (2022)
- [3] A. Nadolska et al., Crystals, 13(6), 905 (2023)

### Acknowledgments

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

## Revealing anisotropic features in structurally isotropic MPX<sub>3</sub> monolayers

M. Rybak<sup>1</sup>, T. Woźniak<sup>2</sup>, P. Scharoch<sup>1</sup> and M. Birowska<sup>1</sup>

<sup>1</sup>*Department of Semiconductor Materials Engineering Faculty of Fundamental Problems of Technology, Wrocław University of Science and Technology Wybrzeże Wyspiańskiego 27, 50-370 Wrocław, Poland.*

<sup>2</sup>*University of Warsaw, Faculty of Physics, Pasteura 5, 00-092 Warsaw, Poland*

Anisotropy is the characteristic feature of a material referring to different physical properties along different directions. Generally, it is an intrinsic property related to atomic structure. The layered materials are naturally anisotropic, as they missing the third dimension. The two-dimensional (2D) materials frequently occurring as an isotropic materials such as widely examined graphene or TMDs. However, the in-plane anisotropy can also occur, or can be induced by various factors such as strain, defects, stacking order, external magnetic or electric fields.

In this work, by used of the density functional theory (DFT), we reveal an occurrence of in-plane anisotropic features in the magnetic, electronic, transport, and optical properties in monolayers of transition metal phosphorus trisulfides (MPX<sub>3</sub>, M=Mn, Ni, Fe, X=S, Se) [1-4]. These materials are 2D antiferromagnetic (AFM) crystals. We have shown, that FePS<sub>3</sub>, exhibit structural anisotropy stemming from breaking of the hexagonal symmetry of magnetic ions, resulting particularly in magnetoelectric anisotropies [1]. Additionally, we have determined the optically active band edge transitions (Mn,Fe)PX<sub>3</sub>, predicting that they are sensitive to in-plane magnetic order [2]. We have revealed linear polarization as an important fingerprints for sensing the type of magnetic AFM arrangements. Additionally, we identify the spin-orientation-dependent features such as the valley splitting, the effective mass of holes, and the exciton binding energy. In particular, we demonstrate that for MnPX<sub>3</sub> (X=S, Se) a pair of non equivalent K<sup>+</sup> and K<sup>-</sup> points exists yielding the valley splittings that strongly depend on the direction of AFM aligned spins. These features can be referred as sensitive parameters that provide insight into spin flop transitions.

### References

- [1] A. Ghosh, M. Birowska, P. Kumar Ghose, M. Rybak, S. Maity, S. Ghosh, B.Das, S. Bera, S. Bhardwaj, S. Nandi, S. Datta, Phys. Rev. B 108, L060403 (2023).
- [2] M. Rybak, P. E. Faria Junior, T. Woźniak, P. Scharoch, J. Fabian, M. Birowska, Phys. Rev. B 109, 054426 (2024).
- [3] R. Basnet, K. Kotur, M. Rybak, C. Stephenson, S. Bishop, C. Autieri, M. Birowska, J. Hu, Phys. Rev. Research 4, 023256 (2022).
- [4] J. Strasdas, B. Pestka, M. Rybak, A. K. Budniak, N. Leuth, H. Boban, V. Feyer, I. Cojocariu, D. Baranowski, J. Avila, P. Dudin, Y. Amouyal, L. Plucinski, E. Lifshitz, M. Birowska, M. Morgenstern, Nano Lett. 23, 10342 (2023)

### Acknowledgments

SONATINA grant, National Science Centre Poland, Magneto-optical properties of two-dimensional magnetic semiconductors and their heterostructures, UMO-2023/48/C/ST3/00309

## Exploring the limits of graphene's operation in extreme conditions imposed by the future energy industry

S. El-Ahmar<sup>1</sup>, W. Reddig<sup>1</sup>, J. Jagiełło<sup>2</sup>, M. J. Szary<sup>1</sup>, A. Dobrowolski<sup>2</sup>, R. Prokopowicz<sup>3</sup>, M. Ziemba<sup>3</sup>, M. Wzorek<sup>2</sup> and T. Ciuk<sup>2</sup>

<sup>1</sup>*Institute of Physics, Poznan University of Technology, Piotrowo 3, 61-138 Poznan, Poland*

<sup>2</sup>*Łukasiewicz Research Network - Institute of Microelectronics and Photonics, Aleja Lotników 32/46, 02-668 Warsaw, Poland*

<sup>3</sup>*National Centre for Nuclear Research, 05-400 Otwock, Poland*

Our research explores the potential of using two-dimensional (2D) carbon structures as magnetic field detectors capable of operating in the extreme conditions of future thermonuclear power plants. In so-called magnetic-confinement fusion reactors, electronics will be exposed to high temperatures and radiation damage. We demonstrate the experimental study on the impact of neutron radiation and determine its influence on the electrical parameters of epitaxial graphene-based systems. We have conducted preliminary research to investigate the impact of high temperature [1] and neutron irradiation [2] separately. For this purpose, we fabricated a hydrogen-intercalated quasi-free-standing (QFS) graphene on semi-insulating 4H-SiC(0001) and 6H-SiC(0001), passivated with an Al<sub>2</sub>O<sub>3</sub> layer [3,4]. The systems were exposed to high-energy neutron fluxes using the MARIA research nuclear reactor.

We theorize that the main factor affecting the QFS properties of graphene in tested systems is the depletion of atoms in the hydrogen layer, based on Hall effect measurements and micro-Raman characterization supported by high-resolution transmission electron microscopy. We have predicted, using density functional theory calculations, that damage to the intercalation lowers carrier concentration in graphene. We anticipate that temperatures above 200°C will facilitate the diffusion of the hydrogen atoms from parts with higher to lower concentrations. This effect can reduce the surface area where intercalation is too low to support the separation of the graphene and improve its QFS properties [2].

Understanding the mechanism of damaging the tested systems by neutron radiation is a key milestone in assessing its suitability for magnetic field detection in harsh environments.

### References

- [1] W. Reddig *et al.*, IEEE Sensors Lett. 7 (2023) 2502204.
- [2] S. El-Ahmar *et al.*, Appl. Surf. Sci. 590 (2022) 152992.
- [3] T. Ciuk *et al.*, Carbon Trends 13 (2023) 100303.
- [4] T. Ciuk *et al.*, Carbon 139 (2018) 776.

### Acknowledgments

This work was supported by the Ministry of Education and Science (Poland) within Project No. 0512/SBAD/2420. The research has received funding from the National Science Centre, Poland, under Grant Agreement No. OPUS 2019/33/B/ST3/02677 and the National Centre for Research and Development, Poland, under Grant Agreement M-ERA.NET3/2021/83/I4BAGS/2022. The M-ERA.NET3 has received funding from the European Union's Horizon 2020 research and innovation programme under Grant Agreement 958174.

## Impact of neutron irradiation on defect-related photoluminescence in layered boron nitride

Ł. Grzegorzółka<sup>1</sup>, J. Iwański<sup>1</sup>, A. K. Dąbrowska<sup>1</sup>, R. Bożek<sup>1</sup>, M. Tokarczyk<sup>1</sup>, A. Korgul<sup>1</sup>, Ł. Murawski<sup>2</sup>, R. Prokopowicz<sup>2</sup>, J. Binder<sup>1</sup> and A. Wysmołek<sup>1</sup>

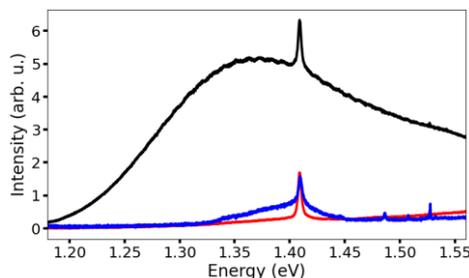
<sup>1</sup>Faculty of Physics, University of Warsaw, Pasteura 5, 02-093 Warsaw, Poland

<sup>2</sup>National Centre for Nuclear Research, Andrzeja Sołtana 7, 05-400 Otwock-Świerk, Poland

Hexagonal boron nitride (hBN) has recently attracted a lot of interest as a candidate for a broad range of applications related to the so-called van der Waals heterostructures, which are composed of thin layers of 2D materials. It has been shown that BN can serve as an excellent host for optically active spin defects, such as negatively charged boron vacancies ( $V_B^-$ ). The extraordinary sensitivity of this defect to perturbations like electric or magnetic field which could be detected by means of ODMR measurements makes it an excellent quantum sensing platform. One of the applications are local magnetic field sensors, which could take the form of an atomically thin film, offering atomic scale proximity to the probed object.

Among different methods aimed to create boron vacancies in BN is irradiation with thermal neutrons. However, thermal neutron flux produced in the nuclear reactor is unavoidably assisted by gamma rays flux and fast neutrons. In addition for the formation of boron vacancies both types of irradiation cause creation of undesired defects which could substantially shorten spin relaxation time, which is crucial for the quantum sensing applications based on  $V_B^-$  in boron nitride.

In this communication we investigate the influence of gamma rays and thermal neutron irradiation on the optical properties of epitaxial layered BN, containing different polytypes such as hBN, rBN or bBN, grown by metalorganic vapour-phase epitaxy (MOVPE). To evaluate the effect of irradiation, we compared Raman and photoluminescence spectra for as-grown and irradiated samples. We found that the position and full-width at half maximum (FWHM) of the  $E_{2g}$  Raman peak are not affected neither by gamma nor by neutron irradiation. On the other hand it was found that both gamma and neutron irradiation influenced defect-related photoluminescence. A new broad band was observed near 1.4 eV for the sample irradiated with neutrons and gamma rays when the sample was illuminated with 785 nm laser (Figure 1). Another band was observed near 1.55 eV when it was illuminated with a 532 nm laser. The changes will be discussed in terms of differences between vacancy defect structure in different polytypes.



**Figure 1.** Photoluminescence spectra of as-grown sample (red), irradiated with gamma radiation (blue) and irradiated with both gamma rays and neutrons (black) excited with 785 nm laser.

### Acknowledgments:

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

## Influence of DUV illumination on the properties of MOVPE grown boron nitride layers

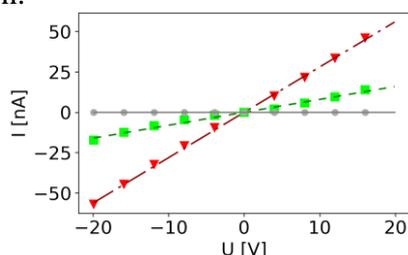
J. Cwynar, A. K. Dąbrowska, J. Iwański, J. Plesiewicz, J. Rogoża,  
J. Binder and A. Wyszmołek

*Faculty of Physics, University of Warsaw, ul. Pasteura 5, 02-093 Warsaw, Poland*

Hexagonal boron nitride (h-BN) is a two-dimensional (2D) material. Due to its wide bandgap (~6 eV) it holds great potential in the area of electronic and optoelectronic structures. An obstacle in this particular field is the lack of efficient n-type and p-type doping, which proves to be essential. A similar issue has been previously encountered in aluminum gallium nitride (AlGaN) where past studies [1] have shown that deep ultraviolet (DUV) illumination (specifically light with energy greater than that of a bandgap) during growth of the material can improve dopant incorporation efficiency. The expectation is that it will affect h-BN in the same way, and so, its potential in optoelectronic applications in the DUV spectral range will be unlocked. Consequently, the aim of this research is to study the effect of DUV illumination on Metal-Organic Vapor Phase Epitaxy (MOVPE) grown h-BN. To this end, the MOVPE system in our laboratory was equipped with an additional optical setup in order to introduce DUV light from high power Laser-Driven Light Source (LDLS) into the reactor.

In this communication, we present the effect of DUV illumination on the optical and electrical properties of h-BN. The impact of illumination was studied during h-BN growth and thermal annealing in nitrogen atmosphere (N<sub>2</sub>) at temperatures of around 1400°C. In order to verify the influence of DUV light on the properties of the grown layers, various characterization techniques were employed, including electrical conductivity, photoluminescence and absorption spectroscopies. We found that the most significant effect was observed for electrical conductivity as presented in Fig. 1. A larger value was observed for annealed samples, which was further increased (by factor of 3) for samples exposed to DUV illumination during the growth. It is an important observation, as it suggests that annealing either enables or activates doping and the DUV light further enhances this effect.

Our findings reveal a significant progress in the field of efficient boron nitride doping. Illumination during growth proved to be a successful means of increasing the conductivity of the material. This finding addresses the long-standing challenge of doping in boron nitride which, if successful, would lead to realizing many potential applications of epitaxial BN in advanced electronic devices. The mechanism responsible for the observed effects will be discussed in this presentation.



**Figure 1.** Measured electric current (I) as a function of applied voltage (U) for different samples: unannealed (circles), annealed (squares) and DUV illuminated and annealed (triangles). The lines represent linear fits.

### References

[1] Z. Bryan et al., Appl. Phys. Lett. 105, 222101 (2014)

## Scanning tunneling microscopy and spectroscopy of nanostructures: from fundamentals to applications

C. Van Haesendonck

*Quantum Solid State Physics, KU Leuven, Celestijnenlaan 200 D, BE-3001 Leuven, Belgium*

With the invention of scanning tunneling microscopy (STM) in 1981 visualizing atoms at a conducting surface became possible. The exponential dependence of tunneling current on distance between tip and sample allows achieving unique vertical and lateral resolution. Essential requirements for reliable STM operation in ultra-high vacuum include reducing vibrational and electronic noise, controlled STM tip motion and positioning, and appropriate surface and tip preparation. Proper interpretation of STM images requires taking into account possible rearrangement of the surface atoms. Scanning tunneling spectroscopy (STS), which relies on measuring the dependence of tunneling current on applied tunneling bias voltage, creates a powerful added value for STM based imaging. STS is not only essential to properly interpret STM images, but moreover provides unique information on the electronic properties.

The application of combined STM and STS at low temperatures can be nicely illustrated using an atomically clean Au(111) surface obtained by epitaxial growth of gold on a mica substrate. First, results will be presented for structural and electronic properties of non-covered Au(111) surfaces. Scattering of the 2D surface state electrons enables quasiparticle interference (QPI) mapping from which the dispersion of the surface states can be inferred. From the QPI maps Fourier transform QPI (FT-QPI) patterns are obtained which directly reflect the Fermi circle of the 2D surface state electrons. Next, results will be presented for Au(111) covered with self-organized nanometer size Co islands grown by deposition of Co atoms. Mapping of the local density of states reveals a strong shape and energy dependence of the electron density variations within the Co islands. Particle-in-a-box calculations enable to reproduce the observed standing wave patterns. Remarkably, standing wave patterns are observed even for high-energy image potential states of electrons that move well above the Co islands. Image potential states have been investigated also for 2D materials and nanostructures of these materials.

When investigating nanostructures that are added on a clean metal surface, it is often necessary to decouple the nanostructures from the underlying metallic surface in order to avoid strong intermixing between the structural and electronic properties of the nanostructures and of the metal. This can be nicely illustrated by covering a Au(111) surface with a few NaCl monolayers on which Au or Co clusters consisting of a limited number of atoms are deposited. For Au clusters, size-dependent sieving behavior occurs with only sufficiently small Au clusters penetrating the NaCl down to the Au(111) support. For Co clusters, size-dependent dissociation of the Co clusters is observed. Decoupling can be realized for 2D materials as well. E.g., graphene on Pt(111) can be decoupled from the Pt(111) by water intercalation.

QPI mapping of the surface of crystals of the topological insulator  $\text{Bi}_2\text{Te}_3$  confirms the expected linear dispersion for the Dirac fermions occupying the 2D topological surface states. FT-QPI patterns further reveal the distribution of the allowed topological surface states in  $k$ -space. Proper identification of native point defects and in situ added Co dopant atoms at the surface of the  $\text{Bi}_2\text{Te}_3$  crystals strongly relies on density functional theory based simulations. Obviously, such an approach can be applied also to defects and dopants in 2D materials.

### Acknowledgments

Where appropriate, references as well as acknowledgements of the involved collaborators will be added for the presented results obtained at KU Leuven.

## Herringbone structures with variable periodicities as the effect of van der Waals Au-Au interactions observed in Au 1 ML on the Ru(0001) surface

I. Morawski, L. Jurczyszyn and M. Nowicki

*Institute of Experimental Physics, University of Wrocław, pl. Uniwersytecki 1, 50-137  
Wrocław, Poland*

In this work we report the formation of reconstructed Au sub-atomic layer adsorbed on the Ru(0001) surface accordingly to the Frenkel-Kontorova herringbone structure model [1] with variable periodicity, which depends on the coverage and the substrate temperature. LEED patterns reveal reconstructed Au layer beginning from low coverages (below 0.1 ML) even at room temperature, though with very low ordering and slight relation to the substrate lattice. The reconstruction order increases at elevated sample temperatures providing sharp satellite spots in LEED pattern, while the periodicity increases with the coverage likewise for the Ag/Ru(0001) interface [2]. At temperatures above  $\sim 300^\circ\text{C}$  and for coverages above  $\sim 0.8$  ML the rapid change from short-period to long-period herringbone structure is observed. The analysis of AES peak intensity during thermal desorption process proves two adsorption energies related to above mentioned periodicities. The DFT calculations show strong influence of Van der Waals interaction between Au atoms on observed superstructures, while the Au – Ru interaction becomes very slight.

### References

- [1] F.C. Frank, J.H. Van der Merwe, Proc. R. Soc. London **198** (1949) 205.
- [2] W.L. Ling et al. Surface Science **600** (2006) 1735.

## Structure of monolayer iron nitride islands on Cu(001) exposed to ambient conditions

W. Andrzejewska<sup>1</sup>, M. V. Dobrotvorska<sup>1</sup>, P. Wojciechowski<sup>1</sup>, Y. Wang<sup>1</sup>, Z. Miłosz<sup>1</sup>, T. Ossowski<sup>2</sup> and M. Lewandowski<sup>1</sup>

<sup>1</sup>*NanoBioMedical Centre, Adam Mickiewicz University in Poznań, Poland, Wszechnicy Piastowskiej 3, 61-614 Poznań*

<sup>2</sup>*University of Wrocław, Institute of Experimental Physics, Max Born Square 9, 50-204 Wrocław*

Iron nitrides exhibit interesting magnetic and electronic properties, making them promising materials for applications in spintronics [1,2]. However, their structural stability under ambient conditions remains unknown. We have studied ultrathin ( $\leq 1$  monolayer-thick) iron nitride islands epitaxially grown on Cu(001) using the well-established procedure, i.e. by bombarding the substrate with low-energy  $N^+$  ions, depositing Fe at room temperature and annealing in ultra-high vacuum (UHV) at 700 K [3,4]. The geometric parameters of the resulting iron nitride, derived from scanning tunneling microscopy (STM) and low energy electron diffraction (LEED) results, matched those of the “Fe<sub>2</sub>N” phase describe in the literature (constituting the middle-plane-cut of the  $\gamma$ -Fe<sub>4</sub>N unit cell [5]). However, the atomic structure exhibited an out-of-plane corrugation that was not reported by other authors so far. Moreover, X-ray photoelectron spectroscopy (XPS) revealed a Fe<sub>1.3</sub>N stoichiometry of the islands, while scanning tunneling spectroscopy (STS) provided a much higher work function value than the one expected for the Fe<sub>2</sub>N phase based on density functional theory (DFT) calculations. On the basis on these findings, we have developed a new structural model for monolayer iron nitride islands on Cu(001), in which an additional layer of (2×2)-arranged N atoms resides on top of the Fe<sub>2</sub>N (resulting in a Fe<sub>1.33</sub>N stoichiometry) [5]. Notably, exposure to ambient conditions was leading to immediate transformation of the islands to iron oxynitride, indicating their low structural stability, but revealing their high potential for catalytic applications.

### References

- [1] T.K. Kim, M. Takahashi, *App. Phys. Lett.* 20 (1972) 492-494.
- [2] Y. Sugita *et al.*, *J. App. Phys.* 70 (1991) 5977-5982.
- [3] Y. Takagi *et al.*, *Phys. Rev. B* 81 (2010) 035422.
- [4] Y. Takahashi *et al.*, *Phys. Rev. Lett.* 116 (2016) 056802.
- [5] J.M. Gallego *et al.*, *Phys. Rev. B* 69 (2004) 121404(R).
- [6] P. Wojciechowski *et al.*, *Vacuum* 220 (2024) 112716.

### Acknowledgments

The studies were financially supported by the Foundation for Polish Science (Polish “Fundacja na rzecz Nauki Polskiej”) through the First TEAM/2016-2/14 (POIR.04.04.00-00-28CE/16-00) project “Multifunctional ultrathin Fe(x)O(y), Fe(x)S(y) and Fe(x)N(y) films with unique electronic, catalytic and magnetic properties” co-financed by the European Union under the European Regional Development Fund. P.W. would like to additionally express his gratitude towards the European Union for the financial support through the European Social Fund Operational Programme “Knowledge Education Development” grant No. POWR.03.02.00-00-I032/16 “Interdisciplinary PhD studies in nanotechnology”. The studies of M.V.D. were supported by the “IDUB support for researchers from Ukraine” project of Adam Mickiewicz University in Poznań. T.O. acknowledges the computer time granted by the ICM of the Warsaw University (projects GB77-16 and GB82-9).

## Investigating polytypism in layered boron nitride using TEM Moiré patterns analysis

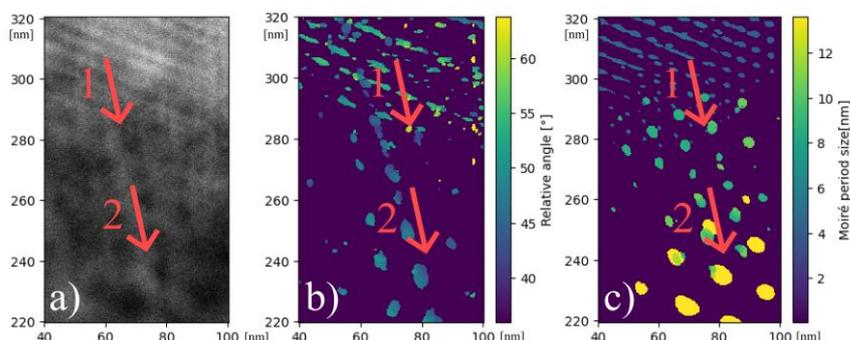
I. Rogala<sup>1</sup>, J. Iwański<sup>1</sup>, A. K. Dąbrowska<sup>1</sup>, S. Kret<sup>2</sup>, J. Binder<sup>1</sup>  
and A. Wyszmołek<sup>1</sup>

<sup>1</sup>Faculty of Physics, University of Warsaw, Pasteura 5, 02-093 Warsaw, Poland

<sup>2</sup>Institute of Physics, Polish Academy of Sciences, Lotników 32/46, 02-668 Warsaw, Poland

Layered boron nitride (BN) exists in the form of various polytypes. Hexagonal boron nitride (hBN) with AA' stacking, rhombohedral boron nitride (rBN) with ABC stacking and Bernal boron nitride (bBN) with AB stacking are among the most interesting. Polytypism in 2D materials seems to be interesting on its own, as effects related to different polytypes, namely piezoelectric effects for non-centrosymmetric polytypes [1] or ferroelectricity [2] are observed. However, what is even more interesting are interlayer twists. Their visible characteristic are Moiré patterns, the analysis of which is the topic of this presentation. While few-atomic layer samples created by stacking of single atomic layers of 2D materials allow for easier formation and control of the specific angles, this is not as straightforward for samples grown via metal-organic vapor phase epitaxy (MOVPE). For samples with thicknesses of many atomic layers determining interlayer angles in such assemblies is a challenge. Thus, a reliable method for analyzing these samples is essential.

Here we present a method for interlayer twist angle and polytype domain identification in scanning transmission electron microscopy (STEM) of MOVPE-grown BN epitaxial layers delaminated onto TEM grid [3] in planar view. Using Fast Fourier Transform we filter the image by Moiré period size and relative angle of Moiré pattern. Then we can distinguish whether a Moiré period change is related to a polytype switching or an interlayer rotation. This approach allows us to map the distribution of these patterns across the sample. Furthermore, this method can be used to optimize sample growth parameters, which is very useful for controlling polytype switching, obtaining single-polytype pure samples, assessing sample quality, identifying dislocations, and determining maximum interlayer angle sizes.



**Figure 1.** STEM image analysis. a) fragment of the STEM image showing the Moiré pattern b) with relative angle map c) Moiré period size map. Arrows mark changes in periodicity of the Moiré pattern. The additional numbering 1) marks a change of the angle and 2) no change of the angle for polytype switching.

### References

- [1] A. Rousseau, et al. Phys. Rev. Mater. 6.9 (2022) 094009.
- [2] Woods, C.R., Ares, P., Nevison-Andrews, H. et al. Nat Commun 12 (2021) 347
- [3] M. Tokarczyk et al. 2D Mater. 10 (2023) 025010

## Electrochemical oxidation of natural graphite as new way of producing a wide range of graphene-based materials

P. Florczak<sup>1</sup>, B. Gurzęda<sup>2</sup>, A. Subrati<sup>1</sup>, M. Kempniński<sup>3</sup>, G. Nowaczyk<sup>1</sup>, E. Coy<sup>1</sup>, J. Jencyk<sup>1</sup>, M. Jarek<sup>1</sup>, L. Smardz<sup>4</sup>, M. Kościński<sup>5</sup>, B. Peplińska<sup>1</sup> and P. Krawczyk<sup>2</sup>

<sup>1</sup>*NanoBioMedical Centre, Adam Mickiewicz University, Wszechnicy Piastowskiej 3, 61-614 Poznań, Poland*

<sup>2</sup>*Institute of Chemistry and Technical Electrochemistry, Poznan University of Technology, Berdychowo 4, 60-965 Poznań, Poland.*

<sup>3</sup>*Faculty of Physics, Adam Mickiewicz University, Uniwersytetu Poznańskiego 2, 61-614 Poznań, Poland*

<sup>4</sup>*Institute of Molecular Physics, Polish Academy of Sciences, Smoluchowskiego 17, 60-179 Poznan, Poland*

<sup>5</sup>*Department of Physics and Biophysics, Faculty of Food Science and Nutrition, Poznan University of Life Sciences, Wojska Polskiego 38/42, Poznań, 60-637, Poland*

Graphite oxide (GO) can be formed by electrochemical oxidation of graphite in aqueous acids. Contrary to the chemical methods electrochemical synthesis is highly controllable, therefore the obtained material is characterized by the desired properties as well composition [1]. GO can be formed by anodic oxidation of graphite in aqueous solutions of perchloric acid. In our research the GO was synthesized from natural graphite flakes by simple one-step anodic oxidation - linear sweep voltammetry. In our research, GO was the starting material for further modifications of this system, one of them was synthesis of bulk quantities of graphene material by the thermal exfoliation–reduction of GO [2]. The second example of these modifications is two-step preparation method of highly oxidized GO flakes with well-ordered layered structure [3]. The third example is intercalation of different types of amines into GO to obtain rigid framework materials [4]. The last series of studies was explanation of impact of oxygen-clustering on the transformation of electrochemically-derived graphite oxide framework [5].

### References

- [1] B. Gurzęda, P. Florczak, M. Kempniński, B. Peplińska, P. Krawczyk, S. Jurga, *Carbon* 100 (2016) 540-545
- [2] B. Gurzęda, P. Florczak, M. Wiesner, M. Kempniński, S. Jurga and P. Krawczyk, *RSC Advances*, 6 (2016) 63058-63063
- [3] B. Gurzęda, A. Subrati, P. Florczak, Z. Kabacińska, T. Buchwald, Le. Smardz, B. Peplińska, S. Jurga, P. Krawczyk, *Applied Surface Science* 507 (2020) 145049
- [4] A. Subrati, P. Florczak, B. Gurzęda, E. Coy, J. Jencyk, M. Kościński, B. Peplińska, S. Jurga, P. Krawczyk, *Carbon* 176 (2021) 327-338
- [5] A. Subrati, B. Gurzęda, P. Jeżowski, M. Kościński, Gr. Nowaczyk, Ma. Kempniński, P. Florczak, B. Peplińska, M. Jarek, Y. Al Wahedi, W. Kempniński, L. Smardz, P. Krawczyk, *Carbon* 217 (2024) 118641

### Acknowledgments

This work was funded by the National Science Centre, Poland (2017/25/B/ST8/01634)

## Graphene-based nanocomposites for applications in radiation protection and thermal management

K. Filak-Mędoń and M. Zdrojek

*Faculty of Physics, Warsaw University of Technology, Koszykowa 75, 00-662 Warsaw,  
Poland*

Graphene-based nanocomposites are becoming emerging materials, offering breakthrough solutions in various fields such as electronics, aerospace, healthcare and defense. The composition of the polymer base and graphene as a filler, forming a nanocomposite, allow also to meet key challenges in the field of radiation protection [1–4] and effective heat management [5,6].

Graphene enhances the ability of nanocomposites to protect against a broad spectrum of electromagnetic radiation, including microwaves, terahertz waves, gamma rays and X-rays. Moreover, the material offers an interesting solution in stealth technologies, offering advanced solutions for absorbing and scattering electromagnetic waves to reduce detectability, achieving a record-low reflection of 0.12%. Graphene-based nanocomposites shield electromagnetic radiation through absorption (more than 20 dB for 10 GHz), keeping their very low reflection coefficient at the same time. Combined with their lightweight nature, these nanocomposites become competitive with currently used high-density materials such as metals, lead, and tungsten. In addition to their electromagnetic shielding capabilities, graphene nanocomposites excel in thermal management. Their high thermal conductivity, exceeding 1.8 W/mK, facilitates efficient heat dissipation, addressing the critical issue of overheating in electronic devices and systems. Interestingly, the anisotropic thermal conductivity of our graphene-based composite allows for directional heat conduction, enhancing the design of materials that direct heat away from critical areas or hot spots.

This presentation will discuss the mechanisms behind the radiation protection of graphene nanocomposites, supported by practical case studies. The potential use of graphene to increase stealth capabilities in military and aviation applications will be indicated. Additionally, directional thermal conductivity will be presented to facilitate effective heat management.

### References

- [1] N. J. AbuAlRoos, et al., *Radiation Physics and Chemistry* **165**, 108439 (2019).
- [2] R. K. Mishra, et al., *Advanced Materials for Electromagnetic Shielding* (Wiley, 2018), pp. 327–365.
- [3] S. Huang, et al., *J. Phys. D: Appl. Phys.* **54**(1), 015001 (2021).
- [4] P. Hillger, et al., *IEEE Trans. THz Sci. Technol.* **9**(1), 1–19 (2019).
- [5] F. Kargar, et al., *Adv Elect Materials* **5**(1), 1800558 (2019).
- [6] K. Zeranska, et al., *ACS Applied Electronic Materials* **4**(9), 4463–4470 (2022).

## Transition metal-doped nickel phosphides on cellulose: efficient electrocatalysts for the oxygen evolution reaction

K. Pietruszewicz, K. Maślana and E. Mijowska

*Department of Nanomaterials Physicochemistry, Faculty of Chemical Technology and Engineering, West Pomeranian University of Technology, Piastow Ave. 45, 70-311 Szczecin, Poland*

For many years, scientists worldwide have concentrated their research efforts on enhancing the current state of our planet. One of the most frequently discussed topics is global warming, which is caused by, among other things, increased carbon dioxide (CO<sub>2</sub>) emissions [1]. Furthermore, the reserves of non-renewable raw materials used as fossil fuels are gradually being depleted as a consequence of increased consumption over time [1].

Concerns about environmental change, particularly concerning greenhouse gas emissions, have led to the pursuit of alternative, renewable energy sources [2], from which hydrogen is considered a promising candidate. H<sub>2</sub> is one of the most pervasive elements in the universe, occurring as chemical compounds (e.g., in water). One method for obtaining molecular hydrogen is the electrochemical splitting of water. The selection of an appropriate electrocatalyst is crucial for performance. Base metals from the d-block appear to offer a promising alternative, given their widespread occurrence and relatively low production costs [2]. The phosphides of these metals display favourable electrochemical activity, high conductivity, corrosion resistance, and stability.

The objective of the research was to synthesise nickel phosphides doped with phosphorus, nickel, and manganese, deposited on carbonized cellulose fibers, and to evaluate their properties in the OER reaction. The products were characterized by various physicochemical methods, such as: TEM, SEM, XPS, XRD, and AAS analysis. The electrochemical tests revealed that obtained catalysts (cel\_Ni<sub>2</sub>P\_Fe10, cel\_Ni<sub>2</sub>P\_Ni10) exhibit an overpotential of 291 mV and 347 mV, which is 17% and 1,4% lower compared to RuO<sub>2</sub>. The presented results confirmed the good stability of all samples. Additionally, the data revealing the mechanism of the reaction are shown.

### References:

- [1] Mustafa Balat, Mehmet Balat, Political, economic and environmental impacts of biomass-based hydrogen, International Journal of Hydrogen Energy, Volume 34, Issue 9, 2009, Pages 3589-3603,
- [2] Xiang, D.; Zhang, B.; Zhang, H.; Shen, L. One-Step Synthesis of Bifunctional Nickel Phosphide Nanowires as Electrocatalysts for Hydrogen and Oxygen Evolution Reactions. Front. Chem. 2021, 9, 773018.

**Acknowledgments:** This research has received funding from National Science Centre (Poland) with grant PRELUDIUM20 number 2021/41/N/ST5/03202.

## **Lanthanoid sesquioxide ultrafine nanoparticles on graphene via general and novel approach of Ultrafast Redox Reaction and their performance as anodes in lithium-ion batteries**

T. Kędzierski<sup>1,2</sup> and E. Mijowska<sup>1,2</sup>

<sup>1</sup> *Department of Nanomaterials Physicochemistry, Faculty of Chemical Technology and Engineering,  
West Pomeranian University of Technology in Szczecin, Piastów 42, 71-065 Szczecin,  
Poland;*

<sup>2</sup> *Center for Advanced Materials and Manufacturing Process Engineering (CAMMPE), West Pomeranian University of Technology in Szczecin, 70-310, Szczecin, Poland.*

Herein, we propose a general route of obtaining reduced graphene oxide and metal oxide nanocomposite, demonstrated by cerium, dysprosium and neodymium sesquioxides, via Ultrafast Redox Reaction (URR). This method utilizes a very fast heating of graphene oxide and a metal salt without any chemical solvents or special reactors. Off the scene tests showed that different ratios of graphene oxide to metal salt change the metal oxide particle size. Morphological, structural, physicochemical and electrochemical properties were investigated. It was proved via XRD and XPS data that it was also possible to oxidize dysprosium acetate and neodymium nitrate at 300°C which normally would require much higher temperatures. As-obtained nanocomposites were tested as anodes in Li-ion batteries but their applications should be further expanded to different fields. As Li-ion anodes they delivered as high capacity as 1173 mAh/g at 0.05 A/g. Interestingly, *ex-situ* measurements of the anode material showed that upon charging ceria is activated to form multiwalled carbon nanotubes. In that respect, we believe that URR route is ultrafast method (lasts in eyeblink emitting colorful sparkles and smoke) to design graphene/metal oxide nanocomposites with tuned nanoparticles size at lower temperatures and without solvents which represents facile and environmentally friendly approach served for various applications.

## **Structural studies of borophene materials by Electron Paramagnetic Resonance technique**

Klaudia Zielinkiewicz, Anna Dymerska, Grzegorz Leniec and Ewa Mijowska

*Department of Nanomaterials Physicochemistry, Faculty of Chemical Technology and Engineering, West Pomeranian University of Technology, Szczecin, Piastów Ave. 45, 71-065 Szczecin, Poland*

Oxygen evolution reaction (OER) and hydrogen evolution reaction (HER) are crucial for renewable energy technologies such as water splitting. Borophene, a two-dimensional (2D) boron material, has attracted considerable interest due to its unique electron deficiency and potential applications in energy conversion. One of the known structural investigation techniques is electron paramagnetic resonance (EPR). The highly sensitive research method allows to study defects in the crystal lattice as well as magnetic ions with unpaired electrons (paramagnetic). EPR analysis reveals insights into the evolution of the chemical structure during the electrochemical process and also deepens the understanding of borophene's electrocatalytic mechanisms, which paves the way for its application in efficient and sustainable energy technologies. The presentation will present the results of ex-situ EPR studies of borophene materials doped with paramagnetic ions, nickel and zirconium. The old technique of EPR studies provides new opportunities to study 2D materials doped with paramagnetic ions.

## On the robustness of gapless states in gated multilayer graphene

W. Jaskólski

*Institute of Physics, Faculty of Physics, Astronomy and Informatics, Nicolaus Copernicus  
University, Toruń, Poland*

Gated multilayer graphene with rhombohedral stacking of layers exhibits a tunable energy gap. The stacking order can be changed when some layers are stretched, or delaminated and corrugated. In such cases, topological gapless states, connecting the valence and conduction band continua, appear at each valley. These states are localized at stacking domain walls (interfaces) that separate two different stacking orders. When the stacking change occurs along the zigzag direction, the Dirac cones at different valleys in the  $k$ -space are well separated. The gapless states are therefore valley-protected and provide one-dimensional and non-destructive valley currents that can flow along the stacking domain wall in opposite directions. Valley protection can be destroyed in the presence of atomic-scale defects. Here, we demonstrate the robustness of the gapless states to different defect-like perturbations of the multilayers. It is shown that some gapless states survive very strong distortions of the stacking domain walls. They persist when some layers are broken or partially removed, or even when vacancies or magnetic impurities are present at the stacking interface.

### References

- [1] W. Jaskólski, M. Pelc, L. Chico, and A. Ayuela, *Nanoscale* 8, 6079, 2016
- [2] W. Jaskólski, *Phys. Rev. B* 100, 035436, 2019
- [3] W. Jaskólski and A. Ayuela, *RSC Advances* 9, 42140, 2019
- [4] W. Jaskólski and G. Sarbicki, *Phys. Rev. B* 102, 035424, 2020
- [5] W. Jaskólski, *Mol. Phys.* e2013554, 2022
- [6] W. Jaskólski, *Solid State Comm.* 360, 115043, 2023
- [7] W. Jaskólski, *Physica E* 157, 115878, 2024

## Proximity induced spin-orbit coupling phenomena in twisted graphene-based van-der-Waals heterostructures

I. Wojciechowska and A. Dyrdał

*Department of Mesoscopic Physics, ISQI, Faculty of Physics, Adam Mickiewicz University in Poznan, ul. Uniwersytetu Poznanskiego 2, 61-614 Poznan, Poland*

The graphene-based van-der-Waals heterostructures reveal fascinating topological and transport phenomena, and therefore are currently extensively investigated as a promising platform for new generation spintronics and electronics. Importantly, proximity effects play a crucial role, enabling the customization of electronic, magnetic, and topological properties of van-der-Waals two-dimensional (2D) materials formed by stacking different 2D crystals. Additionally, by creating a twist between the layers, one obtains an additional possibility to tune the proximity effects, and thus to strongly modify the electronic and topological properties of the whole structure.

In this presentation, we will discuss our recent theoretical study on the proximity-induced spin-orbit coupling phenomena in twisted graphene-based van der Waals heterostructures [1,2]. In principle, we will show how the twist angle modifies the proximity effects in the studied structures, and we will focus on the graphene deposited on both magnetic ( $\text{CrI}_3$ ) and nonmagnetic ( $\text{MoSe}_2, \text{WSe}_2, \text{MoS}_2, \text{WS}_2$ ) 2D crystals. In our analysis, the van-der-Waals structures are modelled by the effective “kp” Hamiltonians derived based on the symmetry considerations and DFT calculations [2-5]. Within the framework of linear response theory, we derive analytical and numerical characteristics describing the intrinsic spin and anomalous Hall effects [4]. Additionally, we will also show how the transport properties depend on the valley-contrasting physics emerging in twisted graphene-based structures.

### References

- [1] I. Wojciechowska and A. Dyrdał, to be published
- [2] I. Wojciechowska, M. Jafari, M. Gmitra and A. Dyrdał, to be published
- [3] Klaus Zollner, Simão M. João, Branislav K. Nikolić, and Jaroslav Fabian, Phys. Rev. B 108, 235166 (2023)
- [4] Y. Li, M. Koshino, Phys. Rev. B 99, 075438 (2019),
- [5] S. Lee, D. J. P. de Sousa, Y.-K. Kwon, F. de Juan, Z. Chi, F. Casanova, and T. Low, Phys. Rev. B 106, 165420 (2022)
- [6] A. Dyrdał and J. Barnaś, 2D Materials 4, 034003 (2017)

### Acknowledgments

This work has been supported by the Norwegian Financial Mechanism 2014-2021 under the Polish-Norwegian Research Project NCN GRIEG “2Dtronics” no. 2019/34/H/ST3/00515.

## Electronic and optical properties of twisted PtSe<sub>2</sub>

P. Jureczko<sup>1</sup> and M. Kurpas<sup>1</sup>

<sup>1</sup>*Institute of Physics, University of Silesia in Katowice, 41-500 Chorzów, Poland*

Monolayer PtSe<sub>2</sub> is a transition metal dichalcogenide semiconductor with an indirect gap and 1T-type crystal structure [1]. Besides promising electrical and optical properties, PtSe<sub>2</sub> exhibits good air stability with high room-temperature carrier mobility and excellent tunability of the band gap by controlling the number of layers [2]. All of this makes PtSe<sub>2</sub> a very promising material for field-effect transistor technology, photodetectors or sensors [3].

Using first principle calculations based on the density functional theory, we study the twist-angle dependence of electronic and optical properties of bilayer PtSe<sub>2</sub>. By examination of the electronic structure and imaginary part of the dielectric tensor, we find that the most significant changes in the dielectric function are observed between 0° and 60° twist angle. In contrast, for twist angles between 13° and 32°, optical properties do not differ much.

We also study the effects of vertical strain on the electronic and optical properties. Our numerical results show that the additional absorption peak occurs at a photon energy of 1eV due to gap reduction in the experimentally accessible strain values [4]. For strains above 2.4GPa, the systems become metallic in the case of 0° and 60° twist angles. To improve the band gap size, we also performed calculations with hybrids functional. The values of band gap sizes and energy of photon absorption increase compared to the Perdew-Burke-Ernzerhof functional.

### References

- [1] Y. Wang et al., Nano Lett. 15, 6 (2015) 101021.
- [2] G. Wang et al., Advanced Materials 33, 1 (2021) 2004070.
- [3] Y. Zhao et al., Advanced Materials 29, 5 (2017) 1604230.
- [4] B. Fülöp et al., Npj 2D Materials and Applications 5, 82 (2021) 101038.

### Acknowledgments

The project is co-financed by the National Center for Research and Development (NCBR) under the V4-Japan project BGapEng.

## Spin waves in a TMD bilayer antiferromagnet

W. Rudziński, A. Dyrdał and J Barnaś

*Faculty of Physics, ISQI, Adam Mickiewicz University in Poznan, ul. Uniwersytetu  
Poznańskiego 2, 61-614 Poznan, Poland*

We have analyzed theoretically and numerically the spectrum of spin waves in two-dimensional bilayer systems of  $VX_2$  ( $X=S, Se, Te$ ) transition-metal dichalcogenides (TMDs) [1]. The Vanadium atoms within individual atomic layers are coupled ferromagnetically. In case of the bilayer system, the exchange coupling between V atoms located in different planes is either ferromagnetic or antiferromagnetic, depending on the type of dichalcogenide (X) atom. We have analyzed the magnon spectra as a function of magnetic anisotropy, external magnetic field applied along the spin direction as well as in the presence of Dzyaloshinskii-Moriya interactions involved e.g. by an inverse-symmetry breaking external electric field or the proximity effect. The spin-wave dispersion relations have been derived analytically within the spin-wave theory, in terms of the Holstein-Primakoff transformation combined with the Bogolubov diagonalization scheme.

The corresponding magnon spectra have been evaluated numerically. In the case of antiferromagnetic TMD bilayers, the system undergoes a field-induced transition to the spin-flop phase, which evolves into the saturated ferromagnetic phase for sufficiently strong magnetic fields. It is shown that existence of different phases depends on the interlayer exchange and anisotropy constants. We have analyzed the spin wave spectra in all these phases and showed how these spectra change at the phase transitions and how they evolve with increasing magnetic field. We have taken into account both, in-plane and out-of-plane magnetic anisotropy as well as in-plane DMI. It is shown that DMI leads to nonreciprocal spin-wave propagation. Moreover, DMI modifies the spin wave spectrum of the bilayers, making its low energy part qualitatively similar to the electronic spectrum of the Rashba spin-orbit model.

The transition of magnetization from in plane to out of plane in  $VSe_2$ - $NiSe_2$  heterostructure [2] led to further discussion on interplay between intralayer nearest-neighbour, next-nearest-neighbour exchange interactions as well as strong out-of-plane magnetocrystalline anisotropy and on its influence on the spin wave-spectra. Due to the proximity effect discussion includes also description of a specific spin-wave behaviour in the presence of Dzyaloshinskii-Moriya interactions.

### References

- [1] H.-R. Fuh, Ch.-R. Chang, Y.-K. Wang, R. F. L. Evans, R. W. Chantrell and H.-T. Jeng, *Scientific Reports* 6, 32625 (2016).
- [2] M. Abdollahi and M. B. Tagani, *Phys. Rev. B* 108, 024427 (2023).

## Revealing active sites and boosting catalytic performance in 2D materials for hydrogen evolution reaction

T. Kosmala

*Institute of Experimental Physics, University of Wrocław, pl. M. Borna 9, 50-204 Wrocław, Poland*

Developing and researching new materials for energy storage and conversion is a top priority in modern scientific research and a crucial challenge in the context of sustainable energy development based on alternative and renewable sources. The efficient conversion of chemical energy into electrical energy and vice versa necessitates the development of innovative electrocatalysts for use in fuel cells, batteries, or electrolyzers. However, current optimization methods primarily rely on the empirical "trial and error" approach, significantly impeding their development.

During this talk, I will showcase some of our recent work on the use of 2D materials in electrochemistry. I will present model systems that have been investigated using advanced in operando and in situ techniques, allowing for the identification of catalytically active sites with atomic precision, along with changes in chemical and electronic states. The presentation will also discuss various strategies for increasing electrocatalytic activity and optimizing catalysts using a knowledge-based approach. I will demonstrate the use of intrinsic defects such as metallic twin boundaries in chalcogenides [1,2], the electron hybridization effect in the Fe/graphene system, and catalysis on single atoms [3] during the presentation.

### References

- [1] T. Kosmala *et al.* Adv. Energy Mater. 8 (2018) 1800031
- [2] M. Lunardon *et al.* ACS Energy Lett. 8 (2023) 972-980
- [3] T. Kosmala *et al.* Nature Catalysis, 4, 10 (2021) 850-859

## Morphological influence on the electrocatalytic efficiency of nickel phosphide and nanocarbon for water electrolysis

K. Maślana, K. Pietruszewicz and E. Mijowska

*Department of Nanomaterials Physicochemistry, Faculty of Chemical Technology and Engineering, West Pomeranian University of Technology in Szczecin, Piastow Ave. 45, 70-311 Szczecin, Poland*

Electrocatalysis is crucial to develop sustainable energy technologies, particularly for efficient water splitting. The efficiency of electrocatalysts is deeply influenced by their structural and morphological characteristics, which dictate their catalytic activity, stability, and overall performance. Traditional precious metal-based catalysts, while effective, are costly and scarce. Thus, there is a pressing need to explore non-precious metal alternatives that offer comparable or superior performance. Recent research underscores the potential of transition-metal-based materials and nanocarbon structures in this domain. Nickel phosphide ( $\text{Ni}_2\text{P}$ ) and nanocarbon materials, including carbon nanotubes, have emerged as promising candidates due to their favorable electronic properties and stability in various reaction environments. Morphological control of these materials is crucial, as it affects the exposure of active sites and the interaction with reactants, thereby influencing the overall catalytic performance.

In response to these challenges, this study investigates the electrocatalytic properties of nickel phosphide ( $\text{Ni}_2\text{P}$ ) and nanocarbon material, focusing on how different morphologies impact HER and OER activities. Our research highlights several key findings: morphological optimization, support effect, innovative catalysts structures and design principle. Prepared electrocatalysts were characterized using various physicochemical methods, including TEM, SEM, XPS, and XRD. The electrochemical properties of the obtained catalysts were examined through electrochemical tests, such as LSV, Tafel slope, Faraday efficiency, and stability, which indicated improved performance compared to  $\text{RuO}_2$ . The reaction mechanism was investigated using both ex situ studies and in situ Raman spectroscopy.

**Acknowledgments** This research has received funding from the National Science Centre (Poland) with grant PRELUDIUM20 number 2021/41/N/ST5/03202.

## Role of MXenes to improve the air stability in perovskite solar cell

S. Sahare<sup>1</sup>, M. Solovan<sup>1</sup>, M. Smirnova<sup>2,3</sup>, B. Scheibe<sup>3</sup> and M. Ziółek<sup>1</sup>

<sup>1</sup>Faculty of Physics, <sup>2</sup>Faculty of Chemistry, and <sup>3</sup>NanoBioMedical Centre, Adam Mickiewicz University, Poznan 61-614, Poland

Hybrid perovskite solar cells (HPSCs) have demonstrated extensive growth in power conversion efficiency (PCE) and cross the power beyond the Si-solar cell technology at the laboratory scale[1]. Despite its stellar performance, the stability of materials and devices is a critical issue instigated by environmental factors such as air, water, and light. These must be addressed before the prospect of PSCs commercialization to compete with traditional Si-solar cell technologies[2]. The 2D material is quite stable, and it has tremendous potential to produce high-performing solar cells with significant stability. Especially, recently developed graphenelike materials, phosphorene, borophene, antimonene, and Mxene played a vital role in HPSCs due to their attractive properties. MXene is an all-rounder 2D material, and its properties such as high absorption, high conductivity, and tuneable work function can be explored in any of the HPSCs components[3]. In this work, the titanium carbide MXene (Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub>) has been introduced in conventional 2D perovskite solar cells as a hole transport interfacial layer. The main objective is to achieve high stability in terms of air and moisture using MXenes. The MXene passivation can modify the interface between the 2D perovskite and hole transport layer, leading to alter the work function, reducing the interfacial impedance, and accelerating the charge 5extractions in the device. These are the foremost causes to enhance the overall performance of PSCs by over 10% than their pristine device. Similarly, the device stability of the device in the air has been demonstrated over 95% for more than 50 days. The increased performance and stability have been analyzed in detail with the help of electrical characterizations and transient absorption spectroscopy, and anticipated the role of MXene in the PSC performance improvement. This work reveals hidden opportunities of MXene as a potential candidate for PSCs and photodetection applications.

**Keywords:** MXene, 2D perovskite, Interface engineering, Stability, Transient absorption spectroscopy.

### References

- [1] Vadakke Neelamana, H., Rekha, S.M. and Bhat, S.V., Chem. Mater. 35(2023) 7386-7405.
- [2] Sahare, S., Pham, H.D., Angmo, D., Ghoderao, P., MacLeod, J., Khan, S.B., Lee, S.L., Singh, S.P. and Sonar, P., Adv. Energy Mater. 11(2021) 2101085.
- [3] Gogotsi, Y. Chem. Mater. 35(2023) 8767-8770.

**Acknowledgments** would like to thank project No. 2021/43/P/ST3/02599 co-funded by the National Science Centre and the European Union's Horizon 2020 research and innovation program under the Marie Skłodowska-Curie grant agreement no. 945339.

## Photoelectrochemical hydrogen evolution utilizing borophene/MoS<sub>2</sub> heterostructure

D. Baranowska, B. Zielińska and E. Mijowska

*Department of Nanomaterials Physicochemistry, Faculty of Chemical Technology and Engineering, West Pomeranian University of Technology, Szczecin, Piastow Ave. 42, 71-065 Szczecin, Poland*

The quest for sustainable energy sources has intensified research efforts toward utilizing solar energy for hydrogen production through photoelectrochemical (PEC) processes. Among various investigated materials, molybdenum disulfide (MoS<sub>2</sub>) has garnered significant attention due to its remarkable electronic and catalytic properties. Moreover, in recent years, the emergence of borophene, a novel two-dimensional (2D) material composed of boron atoms, has opened new avenues for enhancing the performance of MoS<sub>2</sub>-based catalysts. Borophene possesses exceptional electronic properties and tunable band structures, making it an ideal candidate for doping MoS<sub>2</sub> to enhance its PEC activity.

This contribution presents the fabrication, characterization, and application of borophene/MoS<sub>2</sub> heterostructure for efficient hydrogen evolution. The investigations included photocatalytic, electrochemical, and photoelectrochemical hydrogen evolution from water splitting reactions. The structural and electronic properties of borophene/MoS<sub>2</sub> were systematically investigated using advanced characterization techniques, including Transmission Electron Microscopy (TEM), Atomic Force Microscopy (AFM), X-ray Diffraction (XRD), and Raman Spectroscopy.

Evaluating H<sub>2</sub> generation toward borophene/MoS<sub>2</sub> under visible light illumination revealed enhanced hydrogen evolution rates compared to pristine MoS<sub>2</sub> in PEC. Ex-situ studies elucidated the synergistic effect between borophene and MoS<sub>2</sub> unveiling the mechanisms underlying the improved PEC activity. Furthermore, assessing the stability and durability of borophene/MoS<sub>2</sub> catalysts under prolonged PEC operation demonstrated robust performance over extended periods.

This study highlights the potential of borophene/MoS<sub>2</sub> as a promising candidate for efficient solar-driven hydrogen evolution, providing insights into the design and development of advanced catalytic materials for sustainable energy applications. The findings contribute to the ongoing efforts to advance renewable energy technologies and pave the way for commercializing next-generation PEC systems.

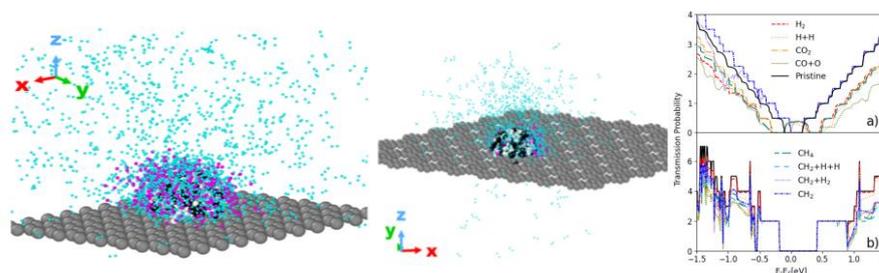
## P1: 2D materials catalysis: a multiscale quantum chemistry approach for hydrogen production from CH<sub>4</sub>, CO<sub>2</sub> purification, and gas splitting applications

A. Aligayev<sup>1,2</sup>, F. J. Dominguez Gutierrez<sup>1</sup>, S. Papanikolaou<sup>1</sup>, Q. Huang<sup>2</sup>

<sup>1</sup>NOMATEN Centre of Excellence, National Centre for Nuclear Research, ul. A. Sołtana 7, 05-400 Otwock, Poland.

<sup>2</sup>Hefei Institute of Physical Science of Chinese Academy of Science, University of Science and Technology of China, Hefei, 230026, China

Two-dimensional carbon-based materials, such as graphene, graphenylene, g-C<sub>3</sub>N<sub>4</sub>, and graphyne, have shown promise for various applications, including electronics, optics, energy storage, and gas separation. Their unique electronic and optical characteristics make them particularly appealing for hydrogen production. In this study, we use computational chemistry models to investigate how methane and carbon dioxide adsorb onto single-layer sheets, focusing on their effects on optical absorption and electrical conductivity at room temperature. To closely mimic experimental conditions, we utilize the self-consistent charge tight-binding density functional theory (SCC-DFTB) [1-5] and validate our findings with ab initio calculations using VASP [2-3]. Through classical molecular dynamics (MD) simulations, we observe hydrogen molecules forming from CH<sub>4</sub> and CO+O species from CO<sub>2</sub> [2,3]. Additionally, we explore how molecular adsorption affects optical absorption. We find that methane and methylene (CH<sub>2</sub>) significantly influence the optical properties of porous carbon sheets, making them favourable for gas diffusion [2-4]. Our MD simulations suggest the potential of porous carbon sheets for gas separation, especially for CH<sub>4</sub>, while CO<sub>2</sub> has a limited impact on the optical properties of these 2D materials [2]. For electron transport analysis, we employ the open-boundary non-equilibrium Green's function method. Studying the conductivity of carbon sheets under voltage bias up to 300 mV provides valuable insights into their electrical properties under optical absorption conditions [2,3]. Our computational modelling results contribute to a better understanding of the potential applications of these materials in hydrogen production and advanced electronics [1,5].



**Figure:** Left panel, visualization of the hydrogen production by graphene and graphenylene. Total transmission probabilities summed over all channels in the nanoribbon graphene direction in a) and through the pores of graphenylene in b).

### References:

- [1] F. Dominguez-Gutierrez, A. Aligayev et al. Phys. Status Solidi B 2200567 (2023)
- [2] A. Aligayev, F. Dominguez-Gutierrez et al. Applied Surface Science (2023)
- [3] A. Aligayev, F. Dominguez-Gutierrez et al. Diamond and related materials (2024)
- [4] C. Liu, A. Aligayev et al. ACS Nano, submitted (2023)
- [5] A. Aligayev, F. Raziq et al. Graphene, Nanotubes and Quantum Dots-Based Nanotechnology, 355–420 (2022)

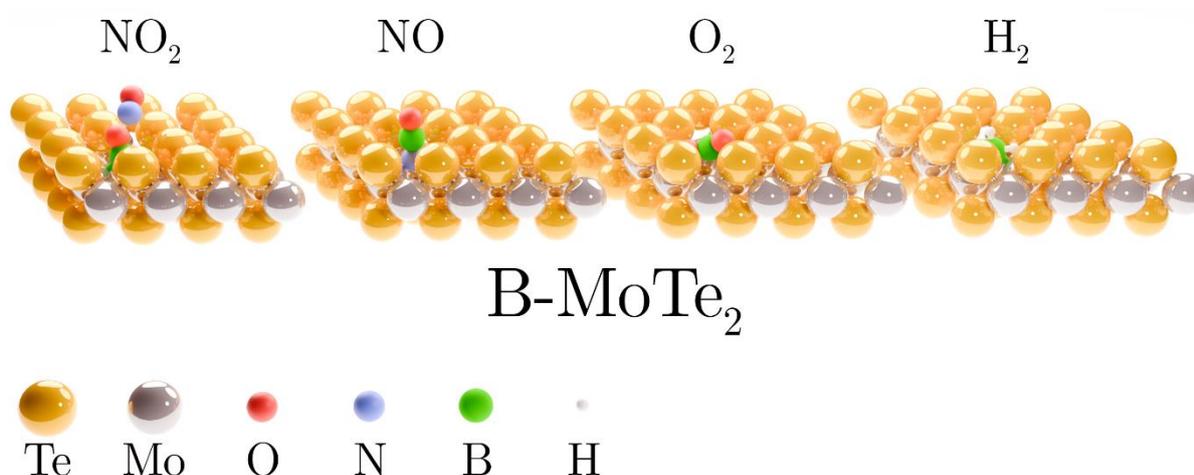
## P2: Demonstration of power of the boron-doped MoTe<sub>2</sub>: computational study of N<sub>2</sub>O, NO<sub>2</sub>, NO, N<sub>2</sub>, CO<sub>2</sub>, CO, O<sub>2</sub>, H<sub>2</sub>O, and H<sub>2</sub> adsorption

P. Radomski<sup>1</sup>, D. Florjan<sup>2</sup>, and M. Szary<sup>2,\*</sup>

<sup>1</sup>*Institute of Materials Research and Quantum Engineering, Poznan University of Technology, ul. Piotrowo 3, 61-138 Poznan, Poland*

<sup>2</sup>*Institute of Physics, Poznan University of Technology, ul. Piotrowo 3, 61-138 Poznan, Poland*

Due to their beneficial electronic and structural properties, monolayers of transition-metal dichalcogenides (TMDs) demonstrate a range of potential applications in electronic and optoelectronic devices, energy storage, and electrocatalysis. Noteworthy among them is MoTe<sub>2</sub>, which shows outstanding high sensitivity in gas detection and can serve as a hydrogen evolution reaction (HER) catalyst. Many of the TMDs best attributes are unlocked only after careful doping. In our previous work [1] we analyzed the effect of 22 p-block dopants on hexagonal MoTe<sub>2</sub> sheet using the methods of density functional theory (DFT). Based on this, we established that by far the greatest activity is shown by the boron-doped layer. Encouraged by the results we present the investigations of its power, judged through the adsorption of 9 commonly encountered molecules: N<sub>2</sub>O, NO<sub>2</sub>, NO, N<sub>2</sub>, CO<sub>2</sub>, CO, O<sub>2</sub>, H<sub>2</sub>O, and H<sub>2</sub>. The results show, that B-MoTe<sub>2</sub> can separate NO<sub>2</sub> → NO + O, as well as break NO, O<sub>2</sub>, and H<sub>2</sub>. Moreover, the boron atom was found to chemically bond with N<sub>2</sub>O, CO, and H<sub>2</sub>O. The interaction with N<sub>2</sub> and CO<sub>2</sub> remained in the domain of physisorption, however, it has still been significantly improved compared to pure MoTe<sub>2</sub>. In general, B-MoTe<sub>2</sub> shows remarkable chemical activity, indicating its possible future applications in catalysis and gas detection.



**Figure 1.** Schematic representation of B-MoTe<sub>2</sub> chemical activity: broken molecules of NO<sub>2</sub>, NO, O<sub>2</sub>, and H<sub>2</sub>.

### References

[8] D. Florjan and M. J. Szary, Acta Materialia 272 (2024) 119951.

### Acknowledgments

This work was supported by the Ministry of Education and Science in Poland (Grant No. 0512/SBAD/2420) within the project realized at the Institute of Physics, Poznan University of Technology. Computations reported in this work have been performed at Poznan Supercomputing and Networking Center (PSNC) under Grant No. pl0093-02.

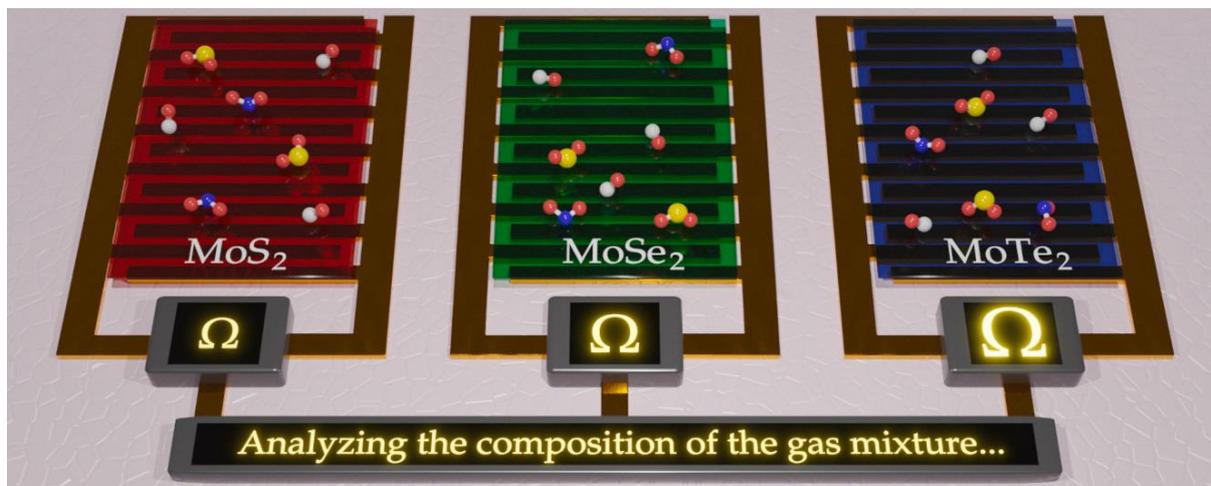
### P3: Toward high selectivity of sensor arrays: selectivity of gas detection on transition metal dichalcogenides

M. J. Szary

*Institute of Physics, Poznan University of Technology, ul. Piotrowo 3, 61-138 Poznan, Poland*

Resistive gas sensors play a crucial role in air quality monitoring, industrial safety, and automotive emission control. Traditional sensing materials often exhibit limited selectivity and require high operating temperatures, reducing their efficiency. This research presents a novel solution by leveraging the unique physicochemical properties of Mo-bearing transition-metal dichalcogenides (TMDs).

Our findings demonstrate that the variable charge availability on TMD surfaces enhances selective adsorption, resulting in marked differences in responses to various molecules, even at room temperature. The TMD monolayers exhibit exceptional relative sensitivity [1-3], particularly to combustion products, surpassing conventional materials like ZnO and TiO<sub>2</sub> by three orders of magnitude under similar conditions. This remarkable variation in responses generates distinct sensing profiles, allowing for effective cross-referencing in sensor arrays [3]. Consequently, TMD-based devices, even in simple configurations, can prevent false positives and determine gas mixture compositions, potentially revolutionizing gas monitoring with advanced lab-on-a-chip solutions.



**Figure 1.** Schematic representation of a TMD-based sensor array, illustrating the principles of its operation.

#### References

- [1] M. J. Szary and P. Radomski, *J. Phys. Chem. C* 127 (43) (2023) 21374-21386.
- [2] P. Radomski and M. J. Szary, *Acta Materialia* 272 (2024) 119949.
- [3] M. J. Szary, *Acta Materialia* 274 (2024) 120016.

#### Acknowledgments

This work was supported by the Ministry of Education and Science in Poland (grant no. 0512/SBAD/2420) within the project realized at the Institute of Physics, Poznan University of Technology, Poland. Computations reported in this work have been performed at Poznan Supercomputing and Networking Center (PSNC) under Grant No. 608.

## **P4: The role of MXene purification and ion intercalation processes in optimizing photocatalytic hydrogen production**

M. Smirnova<sup>1,2</sup>, B. Scheibe<sup>2</sup> and A. Lewandowska-Andralojć<sup>1,3</sup>

<sup>1</sup>*Adam Mickiewicz University, Faculty of Chemistry, Uniwersytetu Poznańskiego 8, 61-614 Poznań, Poland*

<sup>2</sup>*NanoBioMedical Centre AMU, Wszechnicy Piastowskiej 3, 61-614 Poznań, Poland*

<sup>3</sup>*Centre for Advanced Technologies AMU, Uniwersytetu Poznańskiego 10, 61-614 Poznań, Poland*

Transition metal carbides and carbonitrides, known as MXenes, have recently emerged as an outstanding family of two-dimensional (2D) materials characterized by unique combination of remarkable properties, such as excellent conductivity, exceptional hydrophilicity, large electrochemically active surface, and tailored structure. Due to these attributes, MXenes are extensively investigated for variety of applications. Also, they are anticipated to be applied as co-catalysts for solar-driven water splitting in photocatalytic systems. MXenes are expected to replace noble Pt in photocatalysis.

Nevertheless, numerous factors can affect the photocatalytic activity of MXenes. Firstly, the method used for their synthesis and the corresponding purification processes are of predominant importance. Secondly, the exact protocol for preparing the photocatalytic system before conducting photocatalytic tests plays an equally significant role. It is well established that the intercalation agents used during MXene formation influence the distance between MXene monolayers and the stability of their colloidal solution. Consequently, these agents also affect the available surface area of the MXenes and their overall photocatalytic activity.

In our study, we deposited Co cations on model  $Ti_3C_2T_x$  MXene monolayers in the presence of Eosin Y and investigated the hydrogen evolution rate. Notably, the results varied across different samples, influenced by the purification procedures and intercalation agents used. It is well established that the intercalation agents employed during MXene formation influence the spacing between MXene monolayers and the stability of their colloidal solution. Consequently, these agents also impact the available surface area of the MXenes and their overall photocatalytic activity.

We investigated and compared samples of titanium-based MXenes using powder X-ray diffraction, scanning electron microscopy, and Raman spectroscopy. Our findings revealed that the accessibility of the MXene surface to Co catalyst cations is a key factor in achieving an efficient photocatalytic system. In this work, we demonstrate the influence of various parameters on the photocatalytic activity of MXenes in colloidal solutions and determine the optimal conditions for their formation.

### **Acknowledgments**

This work was supported by the National Science Centre (Grant Number: UMO-2021/43/O/ST5/00137).

## **P5: Graphene oxide modified zinc anode to improve cycle stability of zinc ion capacitor**

Y. Hua, Q. Yang, E. Mijowska and X. Chen

<sup>1</sup>*Department of Nanomaterials Physicochemistry, Faculty of chemical Technology and Engineering, West Pomeranian University of Technology, Szczecin, Piastów Ave. 42, 71-065 Szczecin, Poland*

The high energy density of the battery and the high power density of the supercapacitor are combined to form a new energy storage system—Metal ion hybrid supercapacitors. Among them, Zinc ion capacitors (ZICs) has become the most promising safe energy storage device due to higher power density and energy density. Similarly, ZICs also have shortcomings that exist in batteries, such as short circuits caused by zinc dendrites, poor cycling performance, etc. In this work, ZIC was assembled with YP-50 carbon materials as cathode, zinc foil as anode and 3 M zinc sulfate as electrolyte to test its electrochemical performance. In addition, we modify the zinc anode with graphene and compare the performance of bare zinc based ZIC. The modification of the zinc anode with graphene can not only guide the uniform electroplating of zinc ions on the zinc anode to reduce the formation of zinc dendrites, but also reduce the corrosion of the zinc anode, thereby improving the coulombic efficiency and cycle performance of the ZIC.

### **References**

- [4] A. Xia *et al.*, Appl. Surf. Sci. 481 (2019) 852-859.
- [5] L. Kang *et al.*, Adv. Energy Mater. (2018) 1801090.

### **Acknowledgments**

HEDAsupercap under Horizon 2020

## P6: Non-covalent interaction of meso-tetrakis(p-sulfonatophenyl) porphyrin with graphene oxide and reduced graphene oxide

A. Leśniewicz<sup>1</sup> and A. Lewandowska-Andrałojć<sup>1,2</sup>

<sup>1</sup>Faculty of Chemistry, Adam Mickiewicz University, Uniwersytetu Poznańskiego 8, 61-614 Poznań

<sup>2</sup>Center for Advanced Technologies, Adam Mickiewicz University, Uniwersytetu Poznańskiego 10, 61-614 Poznań

Research on nanostructures based on the combination of graphene-based materials and organic dyes is of great importance due to their unique optical, electrical, and spectroscopic properties and their potential applications e.g., in photocatalysis (hydrogen production, pollutant or drugs degradation), solar cells [1].

During photocatalytic processes, a common problem is low efficiency due to inefficient electron transfer. To obtain materials with higher charge separation efficiency, an interesting concept is to combine dye molecules with a graphene sheet, which can act as an electron transporter in the photocatalytic system [2]. In the fabricated nanohybrid, GO/RGO is the matrix for the attached dye molecules, which broaden the light absorption of the nanohybrid towards the visible light range. Efficient electron transport from the excited dye molecule to the GO/RGO sheet can occur in these materials. The properties of the fabricated nanohybrids, and above all the occurring long-lived charge separation state, allow the potential use of such materials in photocatalytic processes [2-3].

The aim of our work was to characterize non-covalent interactions between meso-tetrakis (p-sulfonatophenyl) porphyrin (TSPP) and graphene oxide (GO) (Fig. 1) or reduced graphene oxide (RGO) with the ultimate goal of obtaining material with photocatalytic activity. Additionally, Pluronic® F-127 was employed to increase the stability of the obtained nanohybrids. Non-covalent TSPP/GO and TSPP/RGO nanocomposites were synthesized and characterized by steady-state absorption and emission measurements as well as by time correlated single photon counting.

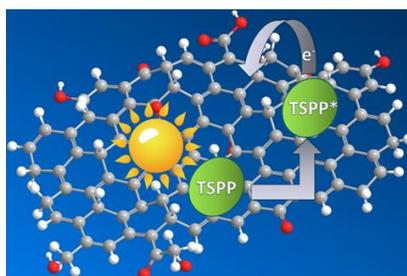


Figure 1. Scheme for non-covalent functionalization of TSPP molecules on GO sheet.

### References

- [6] A. R. Monteiro, M. G. P. M. S. Neves, T. Trindade, ChemPlusChem 85, 1857 (2020).
- [7] J. Albero, D. Mateo, H. García, Molecules 24, 906 (2019).
- [8] X. Li, J. Yu, S. Wageh, A. A. Al-Ghamdi J. Xie, Small 12, 6640 (2016).

### Acknowledgments

This work was supported by the AMU “Excellence Initiative - Research University” (054/13/SNŚ/0025).

## **P7: Nanohybrid systems of m-THPC with Pluronic P123 and graphene oxide: a promising approach for photodynamic cancer therapy**

A. Kolman<sup>1</sup> and A. Lewandowska-Andrałojć<sup>1,2</sup>

<sup>1</sup>*Faculty of Chemistry, Adam Mickiewicz University, Uniwersytetu Poznańskiego 8, 61-614 Poznań*

<sup>2</sup>*Center for Advanced Technologies, Adam Mickiewicz University, Uniwersytetu Poznańskiego 10, 61-614 Poznań*

In this study we have synthesized and characterized nanohybrid systems composed of m-THPC (meso-tetrahydroxyphenylchlorin), Pluronic P123, and graphene oxide (GO) for potential use in photodynamic therapy (PDT). One of the limitations of traditional photosensitizers like m-THPC is their poor solubility and tendency to aggregate in physiological conditions, reducing their effectiveness in PDT. Additionally, graphene oxide tends to aggregate in electrolyte solutions, which can compromise its stability and functionality [1-5].

To address these limitations we have deposited m-THPC on the surface of graphene oxide in the presence of Pluronic P123 which acted as a stabilizing surfactant. UV-Vis absorption spectroscopy was used to analyze the interactions and stability of the nanohybrids. The results demonstrated effective m-THPC adsorption on graphene oxide and significant improvement in stability and solubility in water due to Pluronic P123. Moreover, the spectroscopic characterization confirmed the retention of the photosensitizing properties of monomeric form of m-THPC, suggesting that the obtained nanohybrids could be effective agents in PDT.

In conclusion, the conducted studies indicate that the nanohybrid systems m-THPC/Pluronic P123/GO possess favorable physicochemical and photophysical properties, making them promising candidates for further research on their application in photodynamic therapy for cancer.

### **References**

- [1] Li, D., Müller, M., Gilje, S. et al. *Nature Nanotech* 3, 101–105 (2008).
- [2] Rai, R., Kumar, V. & Pandey, S. *Phys. Chem. Chem. Phys.* 16, 7263–7273 (2014).
- [3] De Napoli, M. et al. *J. Am. Chem. Soc.* 126, 5934–5935 (2004).
- [4] Giovannetti, R., Alibabaei, L. & Petetta, L. *J. Photochem. Photobiol. A. Chem* 211, 108–114 (2010).
- [5] Giovannetti, R., Alibabaei, L. & Pucciarelli, F. *Spectrochim. Acta A Mol Biomol. Spectrosc.* 73, 157–162 (2009).

## P8: Extreme radiation resistance of quasi-2D perovskite solar cells

M. Solovan<sup>1</sup>, H. Parkhomenko<sup>2</sup>, T. Kovaliuk<sup>3</sup>, M. Kaikanov<sup>2</sup> and M. Ziółek<sup>1</sup>

<sup>1</sup>*Faculty of Physics, Adam Mickiewicz University, Poznan 61-614, Poland*

<sup>2</sup>*Department of Physics, School of Sciences and Humanities, Nazarbayev University, Astana 010000, Republic of Kazakhstan*

<sup>3</sup>*Department of Condensed Matter Physics, Faculty of Mathematics and Physics, Charles University, 12116 Prague 2, Czech Republic*

Perovskite has been heralded as one of the most promising emerging materials over the last decade and is extensively used in optoelectronic applications [1]. Perovskite's high absorption coefficient, optimal bandgap, low exciton binding energy, and tolerance to defects have enabled perovskite solar cells (PSCs) to achieve a record efficiency of 26.1% with significant effort and steadily approaching the Shockley–Queisser efficiency limit of 33.7%. However, material stability is a major concern in the prospect of commercialization. Compared to three-dimensional (3D) perovskite materials, two-dimensional (2D) perovskites and quasi-2D perovskites with an increased number of inorganic sheets have attracted increasing attention because of their excellent stability[1]. Currently Zhang Yalan, and Nam-Gyu Park have developed a quasi-2D PSC using a multidimensional hybrid  $\text{GA}(\text{MA})_n\text{PbnI}_{3n+1}$  ( $n = 5$ ) alternating cation perovskite with a PCE of over 22% [2]. At the same time, they also offer cost-effective approaches compared to classical semiconductors because of their solution-processed fabrication methods at low temperatures, directing their employment in portable and wearable electronics, the Internet of Things, and space technologies. It should also be noted that PSC achieves the highest power-to-weight ratio. Based on the above, PSCs are promising for meeting the needs of spacecraft in lightweight energy systems. The space environment poses challenges due to its complexity and variability, subjecting PSCs to harsh conditions such as extreme radiation.

This work investigates the radiation resistance of quasi-2D perovskite solar cells under extreme short-pulse proton irradiation conditions for the first time. The devices were subjected to low energy 170 keV pulsed (150 ns) proton irradiation, with a fluence of up to  $10^{13}$  p/cm<sup>2</sup>, corresponding to approximately 30 years of operation in low Earth orbit. We conducted a complex material characterization of the perovskite active layer and a device physics analysis of the perovskite solar cells before and after short-pulse proton irradiation. The obtained results indicate that the photovoltaic performance of the solar cells experiences a slight deterioration up to 8 % and 43 % following the low  $2 \cdot 10^{12}$  p/cm<sup>2</sup> and high  $1 \cdot 10^{13}$  p/cm<sup>2</sup> proton fluences, respectively, owing to increased recombination losses. It is worth noting that quasi-2D perovskite solar cells show an average of 10% higher than stability compared to traditional 3D triple cation perovskite solar cells under the same irradiation conditions [3].

### References

- [9] T.L. Leung, *et al.*, Commun. Mater. 3 (2022)1–10.
- [10] Y. Zhang and N.-G. Park, ACS Energy Lett. 7 (2022) 757–765.
- [11] H.P. Parkhomenko, *et al.*, Advanced Functional Materials. 34 (2024) 2310404.

### Acknowledgments

M.S. thanks the Polish National Agency for Academic Exchange (NAWA) for financial support within the Ulam NAWA Program (No. BPN/ULM/2021/1/00230).

## **P9: Development of sorption phases with reduced graphene oxide, multiwalled carbon nanotubes and heavy oil fly ash for TF-SPME microextraction and their use for the isolation of PAHs from aqueous matrices**

W. Krumplewski and Iwona Rykowska

*Faculty of Chemistry, Adam Mickiewicz University, Uniwersytetu Poznańskiego 8, 61-614  
Poznań, Poland*

Carbon nanomaterials (CNMs) are characterized by unique physical properties: a very high specific surface area, very high tensile and high temperature mechanical strength, and unique electrical and thermal conductivity. These materials also exhibit high affinity to many organic compounds. The properties allow carbon nanostructures to find their application area in many fields of science and technology, including the usage as adsorption materials<sup>[1]</sup>.

Determination of a wide spectrum of analytes, carried out with analytical instruments in samples with complex matrices, environmental samples included, involves the development of new and selective sorption phases that enable their isolation from different matrices.

Among the sample preparation techniques, solid phase microextraction (SPME) is compatible with green analytical chemistry, as it reduces the use of toxic organic solvents to the minimum. Over the past two decades, this method has undergone impressive progress, resulting in the development of the thin film solid phase microextraction technique (TF-SPME), which is characterized by a much larger surface area of the sorption phase compared to that of the SPME fibre. TF-SPME microextraction instruments, in the form of a mostly rectangular metal or polymer substrate onto which a thin film of sorption phase is applied, are characterized, among others, by a higher sorption capacity. In comparison with microextraction carried out on SPME fibre, they assure faster microextraction of analytes.

Preparation of TF-SPME strips was carried out by dip-coating method. Polydimethylsiloxane (OV-1), cellulose triacetate (CTA) and their dispersions, containing reduced graphene oxide (rGO), multi-walled carbon nanotubes (MWCNT), purified heavy oil fly ash (HOFA) were used as sorption phases. The suitability of the developed microextraction instruments for the concentration and determination of selected PAHs, by gas chromatography, was tested. The subject of the study is related to the kinetics of sorption of analytes from aqueous solutions and their desorption in two organic solvents, namely, acetonitrile and isopropanol. The study made it possible to determine the sorption and desorption times that ensure maximum recovery of analytes in microextractions from aqueous solutions at ambient temperature. For microextraction instruments, with the sorption phase in the form of rGO, MWCNT, and ash dispersed in CTA, the effect of the content of carbon material, in the polymer dispersion, on the recovery of analytes extracted by the TF-SPME technique, was also studied.

### **References**

- [1] Valenzuela, E. F.; de Paula, F. G. F.; Teixeira, A. P. C.; Menezes, H. C.; Cardeal, Z. L. A New Carbon Nanomaterial Solid-Phase Microextraction to Pre-Concentrate and Extract Pesticides in Environmental Water. *Talanta*, **2020**, *217* (January), 121011.

## **P10: Comparison of the excitonic upconversion photoluminescence in MoSe<sub>2</sub> monolayers with a different doping level**

**J. Olejnik<sup>1</sup>, E. Żuberek<sup>1</sup>, J. Łopata<sup>1</sup>, J. Debus<sup>2</sup>, C.-H. Ho<sup>3</sup>, L. Bryja<sup>1</sup> and J. Jadczyk<sup>1</sup>**

<sup>1</sup> *Department of Experimental Physics, Wrocław University of Science and Technology, Wrocław, Poland*

<sup>2</sup> *Department of Physics, TU Dortmund University, 44227 Dortmund, Germany*

<sup>3</sup> *Graduate Institute of Applied Science and Technology, National Taiwan University of Science and Technology, Taipei 106, Taiwan*

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

Here, we compare the UPC PL in an optically bright MoSe<sub>2</sub> monolayer systems revealing different doping level. In hBN-encapsulated MoSe<sub>2</sub> monolayers with a relatively weak electron concentration the UPC PL excitation reveals two pronounced resonances below the neutral 1s A-exciton (X). The resonance detected at an energy of about 25 meV below X coincides with the PL peak and binding energy of the singlet trion TS. The second resonance at –18 meV with respect to the exciton transition is attributed to the neutral biexciton (XX0). The mechanism of the exciton PL upconverted by the neutral biexciton is attributed to the interaction of the photocreated electrons at the K<sup>+</sup> and K<sup>–</sup> valleys with zone-corner flexural acoustic ZA(K) phonons. The UPC of the X PL via the spin-singlet negative trion is assigned to a spin- and valley-conserving scattering process of the photocreated electron with the optical A1 phonon mode whose energy at the K valleys matches the energy difference between the singlet trion and the neutral exciton [1].

Interestingly, in uncapped MoSe<sub>2</sub>/hBN structures with the higher electron density the exciton UPC PL is hardly detected, whereas in hBN/MoSe<sub>2</sub>/graphene/hBN heterostructures, where the doping by resident charge carriers is completely neutralized and results in a vanishing trion emission, the UPC energy gain is about 17 meV and resonates with the energy of the zone-corner flexural acoustic ZA(K) phonon mode.

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

### **References**

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

## P11: Upconversion photoluminescence of a defect-bound exciton in hBN-encapsulated MoS<sub>2</sub> monolayers

E. Żuberek<sup>1</sup>, J. Olejnik<sup>1</sup>, J. Łopata<sup>1</sup>, J. Debus<sup>2</sup>, C.-H. Ho<sup>3</sup>, L. Bryja<sup>1</sup> and J. Jadczyk<sup>1</sup>

<sup>1</sup>*Department of Experimental Physics, Wrocław University of Science and Technology, Wrocław, Poland*

<sup>2</sup>*Department of Physics, TU Dortmund University, 44227 Dortmund, Germany*

<sup>3</sup>*Graduate Institute of Applied Science and Technology, National Taiwan University of Science and Technology, Taipei 106, Taiwan*

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

Here, we demonstrate upconversion (UPC) photoluminescence (PL) of a defect-localized exciton X<sub>L</sub> in hBN/MoS<sub>2</sub>/hBN structures with a high energy gain of about 292 meV at 7 K. The upconverted PL is observed only for samples in which the prominent X<sub>L</sub> line dominates the neutral exciton X in low-temperature PL spectra. Furthermore, we evaluate the UPC PL dependence on changes in the excitation energy, incident laser power and temperature. The intensity of upconverted X<sub>L</sub> transition decreases with decreasing laser excitation energy, reflecting the shape of the lower energy flank of the X<sub>L</sub> PL line, whereas its dependence on the laser power is sub-linear. We propose that the energy gain required in the UPC of the defect-bound exciton PL originates from an electron Auger recombination between in-gap defect defect states introduced by chalcogen vacancies.

[1] E. Żuberek, M. Majak, J. Lubczyński et al., *Sci Rep* **12**, 13699 (2022).

[2] Y. Zhao, M. Tripathi, K. Čerņevičs et al., *Nat Commun* **14**, 44 (2023).

[3] Y. Zhu, J. Lim, Z. Zhang et al., *ACS Nano* **17** (14), 13545-13553 (2023).

**P12: Biopolymers based paper coating with promoted grease resistivity, biodegradable and mechanical properties**

K. Wenelska<sup>1</sup>, T. Kędzierski<sup>1</sup>, K. Maślana<sup>1</sup>, K. Sielicki<sup>1</sup>, A. Dymerska<sup>1</sup>, J. Janusz<sup>2</sup>, G. Mariańczyk<sup>2</sup>, A. Gorgon-Kuza<sup>2</sup>, W. Bogdan<sup>2</sup> and E. Mijowska<sup>1</sup>

<sup>1</sup> *West Pomeranian University of Technology in Szczecin, Faculty of Chemical Technology and Engineering, Department of Nanomaterials Physiochemistry, Piastow Ave. 45, Szczecin, 70-310, Poland*

<sup>2</sup> *Arctic Paper Kostrzyn SA, ul. Fabryczna 1, Kostrzyn nad Odra, 66-470, Poland*

The dominance of plastics in the packaging market is due to their low weight and thickness, which save transportation costs. However, their non-biodegradability poses a significant threat to the environment. Paper, on the other hand, is considered as a safer alternative due to its natural composition and biodegradability. The porous structure of paper limits its application in packaging, and its poor water resistance further restricts its use in humid environments. Therefore, lamination is a method useful tool to improve the barrier properties of paper. Additionally, the researchers are focusing on developing biodegradable and water-based coatings with anti-fat properties as a green alternative to plastic packaging. The impact of a new grease-resistant coating composed of starch, gelatin and sodium alginate on the mechanical properties of paper was investigated through tensile, tearing, and bursting strength tests. The results showed significant improvements in the mechanical properties of the coated paper sheets. Furthermore, the biodegradability test indicated that the paper samples coated with the new composition showed a 50% weight loss after one week of incubation in the soil, and after three weeks, they exhibited 100% weight loss, demonstrating their outstanding biodegradability.

### **P13: Optimizing paper properties with various inorganic crosslinkers for enhanced filler retention**

K. Maślana<sup>1</sup>, K. Sielicki<sup>1</sup>, K. Wenelska<sup>1</sup>, T. Kędzierski<sup>1</sup>, J. Janusz<sup>2</sup>, G. Mariańczyk<sup>2</sup>, A. Gorgon-Kuza<sup>2</sup>, W. Bogdan<sup>2</sup>, B. Zielińska<sup>1</sup> and E. Mijowska<sup>1</sup>

<sup>1</sup>*Department of Nanomaterials Physicochemistry, Faculty of Chemical Technology and Engineering, West Pomeranian University of Technology in Szczecin, Piastow Ave. 45, 70-311 Szczecin, Poland*

<sup>2</sup>*Arctic Paper Kostrzyn SA, ul. Fabryczna 1, 66-470 Kostrzyn nad Odra, Poland*

Achieving desired paper properties such as strength, durability, and printability remains a significant challenge in the papermaking industry. Calcium carbonate (CaCO<sub>3</sub>) is commonly used as a filler to enhance brightness, opacity, and printability. However, weak interactions between cellulose fibers and CaCO<sub>3</sub> particles can lead to issues such as poor folding, tearing, and increased energy consumption due to longer drying times. To address these challenges, this study explores the use of various inorganic additives as crosslinkers to improve the interaction between cellulose fibers and CaCO<sub>3</sub>.

We investigated the effects of mesoporous SiO<sub>2</sub> nanospheres, TiO<sub>2</sub> nanoparticles, h-BN nanoflakes, and hydroxylated h-BN nanoflakes (h-BN-OH) as inorganic filler content in paper. These additives were introduced into the paper pulp as a polyethylene glycol (PEG) suspension to facilitate bonding between the inorganic particles and the cellulose fibers. Detailed microscopic and structural analyses, including transmission and scanning electron microscopy (TEM and SEM), X-ray diffraction (XRD), Raman spectroscopy, and N<sub>2</sub> adsorption/desorption isotherms, were employed to characterize the modified paper samples. The ash content was evaluated following ISO 1762:2001 guidelines to determine the efficiency of filler retention.

Our findings revealed that SiO<sub>2</sub> nanoparticles were the most effective crosslinker, enhancing filler retention by approximately 12.1% compared to unmodified paper sheets. This improvement is attributed to the ability of SiO<sub>2</sub> to form covalent bonds with both cellulose fibers and CaCO<sub>3</sub> particles, thereby strengthening the inter-fiber bonding and improving the overall properties of the paper. Consequently, incorporating inorganic crosslinkers, especially SiO<sub>2</sub> nanoparticles, offers a promising approach to optimize paper properties by enhancing filler retention and improving the interaction between cellulose fibers and CaCO<sub>3</sub> particles. These findings offer valuable insights for the papermaking industry, aiming to produce higher-quality paper products with better performance characteristics.

**Acknowledgments** This research received funding from the National Centre for Research and Development (Poland): POIR.01.01.01-00-0272/19-00.

## **P14: Fabrication and characterization of 2D heterostructure based on MoSe<sub>2</sub> and borophene**

P. Sać, J. Woronowska, D. Baranowska and E. Mijowska

*West Pomeranian University of Technology in Szczecin,  
Faculty of Chemical Technology and Engineering,  
Department of Nanomaterials Physicochemistry, Piastow Ave. 42, 71-065 Szczecin*

Molecular hydrogen (H<sub>2</sub>) is an excellent source of energy due to its high energy density and being environmentally friendly which stems from the fact that the only product of burning hydrogen is water vapor. Considering that the best electrocatalysts for HER (Hydrogen Evolution Reaction) and PEC (Photo-Electrocatalysis) reactions are rare and expensive platinum and palladium, electrochemically stable and abundant materials are considered viable alternatives. 2D-transition metal dichalcogenides (TMDs), which consist of a single layer of TMD, have been studied due to their high-performance in electrochemical water splitting, however only the edge sites of their trigonal prismatic phase show electrochemical activity while the saturated basal plane is inactive. This contribution focuses on the 2D heterostructure of MoSe<sub>2</sub> and borophene composite in view of different mass ratios of the composite components. The goal is to increase the number of electrocatalytic sites by exfoliation of MoSe<sub>2</sub> and borophene flakes. Borophene recently gained a lot of attention as a 2D material due to its incredible properties such as superconductivity and great potential in bridging large-bandgap TMDs. MoSe<sub>2</sub> and borophene composite was synthesized by mechanically stirring in zirconia ball mill, components were stirred for 6 hours at 450 rpm. Samples were optimized, prepared and categorized based on the mass ratios of MoSe<sub>2</sub> to borophene (1:10, 1:1, 10:1 and 100:1). To properly characterize the structure, a variety of techniques have been used, including Atomic Force Microscope (AFM), X-Ray Powder Diffraction (XRD), Raman spectroscopy and Transmission Electron Microscope (TEM).

The results show that out of all synthesized composites, MoSe<sub>2</sub>/B\_1:1 show the most promising results. TEM images show reduced aggregation compared to that of MoSe<sub>2</sub> and other composites. AFM data shows that the thinnest flakes are observed in MoSe<sub>2</sub>/B\_100:1 but their sizes vary substantially, however MoSe<sub>2</sub>/B\_1:1 flakes are also relatively thin while having more uniform sizes. XRD patterns of composite materials have broader and reduced peaks, that indicate the exfoliation of MoSe<sub>2</sub>/B flakes which correlates to the reduction of their crystallinity.

To summarize, this contribution focuses on MoSe<sub>2</sub> and borophene heterostructure as a potential addition to the list of hydrogen fuel generators due to its promising electrocatalytic properties which are a result of increasing the number of electrochemically active edge sites by exfoliating MoSe<sub>2</sub> and borophene flakes.

**P15: Proximity spin-orbit effects in hybrid 1D/2D heterostructures.**

M. Kurpas<sup>1</sup>, M. Milivojević<sup>2,3</sup> and M. Gmitra<sup>4,5</sup>

<sup>1</sup>*Institute of Physics, University of Silesia in Katowice, 41-500 Chorzów, Poland*

<sup>2</sup>*Institute of Informatics, Slovak Academy of Sciences, 84507 Bratislava, Slovakia*

<sup>3</sup>*Faculty of Physics, University of Belgrade, 11001 Belgrade, Serbia*

<sup>4</sup>*Institute of Physics, Pavol Jozef Šafárik University in Košice, Park Angelinum 9, 04001 Košice, Slovakia*

<sup>5</sup>*Institute of Experimental Physics, Slovak Academy of Sciences, Watsonova 47, 04001 Košice, Slovakia*

We study proximity effects in a hybrid heterostructure build of a one-dimensional (1D) carbon nanotube and a 2D material/bulk surface with strong spin-orbit coupling. We show, by performing first-principles calculations, that Dirac electrons in the nanotube acquire large, meV range, spin-orbit coupling due to a close vicinity of the substrate. The calculated low-energy band structure and spin texture of the proximized nanotube display a strong dependence on the position of the nanotube on the substrate, similar to twist-angle dependence found in 2D heterostructures. Dirac states exhibit almost perfect spin polarization, transverse to the nanotube axis and to the stacking direction, forming a proper condition for charge-to-spin conversion with coherent spin transport in the nanotube. Based on the first-principles results, we formulate an effective low-energy Hamiltonian of the nanotube and identify key interactions governing the proximity spin-orbit coupling.

**References**

1. Marcin Kurpas, Phys. Rev. B 108 (2023), 195408.
2. M. Kurpas, M. Milivojević, M. Gmitra (to be submitted).

**Acknowledgments**

The project is co-financed by the National Center for Research and Development (NCBR) under the V4-Japan project BGapEng V4-JAPAN/2/46/BGapEng/2022.

## **P16: Photo-electrochemical characterization of 2D heterostructure based on MoSe<sub>2</sub> and borophene**

J. Woronowska, P. Sać, D. Baranowska and E. Mijowska

*West Pomeranian University of Technology in Szczecin, Faculty of Chemical Technology and Engineering,  
Department of Nanomaterials Physicochemistry, Piastow Ave. 42, 71-065 Szczecin*

Rapidly developing technology as well as the economy have led scientists and researchers to search for new improved energy sources. Their main goal is to design new energy source to reduce CO<sub>2</sub> emissions and discover alternative sources of renewable energy. The most cost-effective way to realize it is the photo-electrocatalytic process. Therefore, this contribution presents a characterization of the influence of the physicochemical properties of dichalcogenide composite structures on their electrocatalytic and photo-electrocatalytic activity in electrochemical water decompositions (Hydrogen Evolution Reactions).

The proposed results are focused on heterostructure based on molybdenum diselenide and borophene. The fabrication route of the composites was carried out in a zirconia ball mill for 6 hours at 450 rpm. In order to reveal the most optimal and effective ratio of, 5 samples with different weight ratio of MoSe<sub>2</sub> to borophene were prepared: 1:10, 1:1, 10:1, 100:1 and 1000:1.

The molybdenum diselenide/borophene composites were subjected primarily to HER (hydrogen evolution reaction) and PEC (photoelectrocatalysis) reactions. In order to gain an in-depth understanding of the electrochemical properties of this material, several techniques were used in both reactions: Linear Sweep Voltamperometry (LSV), Galvanostatic Electrochemical Impedance Spectroscopy (GEIS), Tafel slope analysis and Advanced Cyclic Voltammetry (CVA). The results indicate that the MoSe<sub>2</sub>/B 1:1 sample shows the lowest overpotential in the PEC reaction (-200.58 mV). In addition, it is also distinguished by the lowest Tafel slope, the highest mobility of generated carriers and the highest ECSA. Thanks to Stability Test, it is concluded that it also shows satisfactory stability in acidic environments.

In conclusion, the studies performed clearly show that borophene has a positive effect on the electroactivity of molybdenum diselenide. This effect is observed for both: HER and PEC reactions. The MoSe<sub>2</sub>/B 1:1 sample shows promising results giving alternative strategy to develop hydrogen technology.

## P17: Machine Learning assisted approach for prediction of the g factors of TMDs heterobilayers

K. Gałązka<sup>1</sup>, M. Marchwiany<sup>2</sup>, T. Woźniak<sup>1</sup> and M. Birowska<sup>1</sup>

<sup>1</sup>University of Warsaw, Faculty of Physics, Pasteura 5, 00-092 Warsaw, Poland

<sup>2</sup>Interdisciplinary Centre for Mathematical and Computational Modelling (ICM), University of Warsaw, Pawińskiego 5a, 02-106 Warsaw, Poland

Continued progress of technology and industry necessitates the development of tailor-made materials for specific purposes. In recent years the vast class of two-dimensional (2D) van der Waals (vdW) layered materials have been extensively studied. Among them, Transition Metal Dichalcogenide (TMD) semiconductors have been subjects of particular interest in electronics and optoelectronics. [1]

In principle desired properties could be obtained by vertically stacking various types of monolayer (ML) crystals with arbitrary material sequence and twist angle between layers, owing to their synergistic effects. [2,3] Although the interest in this pursuit is continuously increasing, the lack of high-throughput techniques for fabricating high-quality vdW heterostructures (HTs) hinders its research. The speed of the process could be expedited with the use of theoretical calculations to predict promising structures with desired properties. The  $g$  factor that quantifies the response of excitons to external magnetic field is one of such a property, that has been widely studied in the framework of the density functional theory for MLs of TMDs. [3] However,  $g$  factor research for HTs are limited due to requirement of large number of conduction bands to achieve convergence. [3] Additionally, the stacking layers and twist angles dependence further complicate the research.

This high computational demand and labor intensive process of prediction limits the pace of progress in the field. Many TMD monolayer phenomena have been extensively examined in relation to the  $g$  factor. Namely, experimental studies of exciton complexes, excited Rydberg states etc., and theoretical computations based on electronic structure features. The idea is to investigate and utilise their predictive power using Machine Learning Methods (MLMs), applying this knowledge to TMD vdW HTs.

At first an experimental database was constructed, where all available data from publications was collected and considered. It was then cleaned, all damaged or incomplete records were removed or completed and descriptors of records were established. Next a variety of Decision Tree Regressor based algorithms were fitted to the data. This yielded unsatisfactory results, owing mainly to large inconsistencies between publications and an insufficient amount of published data. Hence, another approach is investigated by creating a dataset based on high throughput *ab initio* computations of TMDs-based alloys.

### References

- [1] J. Qi *et al.*, Int. J. Extrem. Manuf. 5 (2023) 022007.
- [2] K. S. Novoselov *et al.*, Science 353 (2016) 6298.
- [3] T. Woźniak *et al.*, Phys. Rev. B 101 (2020) 235408.

### Acknowledgments

SONATINA grant, National Science Centre Poland, Magneto-optical properties of two-dimensional magnetic semiconductors and their heterostructures, UMO-2023/48/C/ST3/00309

## **P18: Refinement and optimization strategies for the transfer and hierarchical stacking of graphene films**

Q. Yang, Y. Hua, E. Mijowska and X. Chen

*Department of Nanomaterials Physicochemistry, Faculty of chemical Technology and Engineering, West Pomeranian University of Technology, Szczecin, Piastów Ave. 42, 71-065 Szczecin, Poland*

The atomic ultrathin properties of two-dimensional graphene films have great prospects in many applications. In particular, its excellent transparency and excellent mechanical properties endow graphene film with great potential as a supporting layer for nanomaterials. Chemical vapor deposition (CVD) growth of graphene on metal substrates provides tantalizing opportunities for the large area synthesis of graph in a controllable manner. However, there are still great challenges to obtain large-area and high integrity two-dimensional graphene films. Here, centimeter sized graphene films are efficiently transferred to arbitrary substrates to fabricate large-area and high-quality two-dimensional graphene films. By controlling the interfacial force during the transfer process, the integrity of graphene film can be as high as 95%, which is significantly larger than the value reported in previous work. A multilayer graphene film can be formed between single-layer graphene films by  $\pi$ - $\pi$  stacking, which can be used for liquid encapsulation and provide strong support for samples. This simple and scalable preparation of clean and high-quality large-area graphene films is expected to be widely used in electron and optical microscopy.

### **References**

- [2] Zang, X. et al. Graphene and carbon nanotube (CNT) in MEMS/NEMS applications. *Microelectronic Engineering* (2015), 132, 192–206.
- [3] Castellanos-Gomez, A. et al. Mechanics of freely - suspended ultrathin layered materials. *Annalen der Physik* (2015), 527(1-2), 27–44.
- [4] Lu, X. B. et al. Superconductors, orbital magnets and correlated states in magic-angle bilayer graphene. *Nature* (2019), 574(7780), 653.
- [5] Weber, P. et al. Force sensitivity of multilayer graphene optomechanical devices. *Nature Communications*(2016),7.

### **Acknowledgments**

The authors thank Yumeng Hua for her help in Raman spectroscopy characterization. This work was supported by the Plastic Waste Recycling, towards high-porous carbon nanomaterials for Electrochemical Energy Storage project, UPOS,UMO- 2020/39/B/ST8/02937.

## **P19: Synthesis and characterization of free-standing-like antimonene monolayer on silicon**

**M. Gołębiowski, P. Drózdź, M. Jałochowski, M. Kopciuszyński, M. Krawiec and R. Zdyb**

*Institute of Physics, Maria Curie-Skłodowska University, pl. Marii Curie-Skłodowskiej 1, 20-031 Lublin*

The synthesis of two-dimensional materials on various substrates is still a challenge due to numerous factors that must be fulfilled. The material formed on the substrate must not bind too strongly to avoid a chemical compound formation. On the other hand, it cannot bind too weakly, as it must be stable. In addition, immiscibility, thermal stability and matching of the lattice constant play a significant role. Antimonene has been synthesized so far on substrates such as SiO<sub>2</sub>, PbTe<sub>2</sub>, Ge(111), Ag(111), Cu(111) and Cu(110), however, in a form of nanoflakes or islands of submillimeter size [1].

In this report, we present a single layer of antimonene synthesized on a silicon surface, bounded with the substrate via van der Waals interaction. Studies performed with LEEM/LEED (Low Energy Electron Microscopy/Diffraction), STM (Scanning Tunneling Microscopy) and ARPES (Angle-Resolved Photoemission Spectroscopy) techniques reveal that the synthesized two-dimensional Sb shares many features with theoretical models of a single layer of free-standing antimonene.

Antimony was deposited by molecular beam epitaxy (MBE) on Si(111)-(6x6)Au substrate under ultra-high vacuum (base pressure  $3 \cdot 10^{-10}$  mbar) conditions. LEED studies revealed the honeycomb structure formation belonging to beta phase antimonene. The determined lattice constant of the resulting 2D material is  $4.08 (\pm 0.08)$  Å and fits perfectly to the lattice constant predicted by theoretical calculations [2,3].

The growth of antimonene traced in LEEM is consistent with the Stransky-Krastanov mechanism. Deposited Sb prefers defects on the substrate surface as nucleation sites. In both LEEM and STM, it was observed that the irregular shape of the formed islands does not reflect the symmetry of substrate crystallographic structure, which may suggest a weak bonding in the interface. Indeed, the STM reveals that the height of the islands is  $4.4 (\pm 0.1)$  Å, which indicates their weak interaction with the substrate. The completed monolayer tightly covers the surface of the substrate with a cm<sup>2</sup> size.

ARPES maps show that the band structure of the antimonene single layer is very similar to that obtained from the DFT calculations made for free-standing antimonene, which also indicates weak bonding to the substrate [4]. In addition, the absence of electron bands near the Fermi level implies the semiconductive nature of the created antimonene monolayer.

### **References**

- [6] D. Zhou *et al.* Adv. Funct. Mater. **31** (2021) 2006997
- [7] X. Wang *et al.*, Appl. Surf. Sci. **491** (2019) 451-459
- [8] X. Chen *et al.*, J. Mater. Chem. C **4** (2016) 5434-5441
- [9] S. Zhang *et al.*, Angew. Chem. Int. Ed. **54** (2015) 3112-3115

### **Acknowledgments**

The research was carried out as part of the research project of the National Science Center No. 2020/37/B/ST5/03540.

## **P20: Atoms near graphene nanoantennas: interplay of optical coupling and electron tunneling**

M. Kosik<sup>1</sup>, M. M. Müller<sup>2</sup>, K. Słowik<sup>1</sup>, G. Bryant<sup>3</sup>, A. Ayuela<sup>4</sup>, C. Rockstuhl<sup>2, 5</sup>  
and M. Pelc<sup>1</sup>

<sup>1</sup>*Institute of Physics, Nicolaus Copernicus University in Toruń, Grudziądzka 5/7, 87-100 Toruń, Poland*

<sup>2</sup>*Karlsruhe Institute of Technology, Institute of Theoretical Solid State Physics, Kaiserstr. 12, 76131 Karlsruhe, Germany*

<sup>3</sup>*Joint Quantum Institute, University of Maryland and National Institute of Standards and Technology, College Park 20742, MD, USA; Nanoscale Device Characterization Division, National Institute of Standards and Technology, Gaithersburg 20899, MD, USA*

<sup>4</sup>*Centro de Física de Materiales, CFM-MPC CSIC-UPV/EHU, Paseo Manuel Lardizabal 5, Donostia-San Sebastian 20018, Spain; Donostia International Physics Center (DIPC), Paseo Manuel Lardizabal 4, Donostia-San Sebastian 20018, Spain*

<sup>5</sup>*Karlsruhe Institute of Technology, Institute of Nanotechnology, Kaiserstr. 12, 76131 Karlsruhe, Germany*

Graphene flakes acting as photonic nanoantennas may sustain strong electromagnetic field localization and enhancement. To exploit the field enhancement, quantum emitters such as atoms or molecules should be positioned in such close proximity to the flake that electron tunneling might influence the optical and electronic properties of the system. However, tunneling is usually not considered if the optical coupling mechanism between quantum emitters and nanoantennas is at focus. Here we present a framework for describing the electron dynamics in hybrid systems consisting of graphene nanoflakes coupled both electronically and optically to adatoms and subject to external illumination. Our framework combines the single-particle tight-binding approach with a nonlinear master equation formalism that captures both optical and electronic interactions. We apply the framework to demonstrate the impact of electron tunneling between the adatom and the flake on emblematic quantum optical phenomena: degradation of coherent Rabi oscillations and quenching of Purcell spontaneous emission enhancement in two-level adatoms in proximity of triangular graphene nanoflakes.

GRAPHENE  
& 2D Mat  
POLISH CONFERENCE



# List of Participants

**Amil Aligayev**

National Centre for Nuclear Research, Poland  
Poster presentation

**Weronika Andrzejewska**

Adam Mickiewicz University in Poznań, Poland  
Oral presentation

**Subrahmanyam Bandaru**

University of Warsaw, Poland  
Oral presentation

**Daria Baranowska**

West Pomeranian University of Technology, Poland  
Oral presentation

**Józef Barnaś**

Adam Mickiewicz University in Poznań, Poland  
Regular Participant

**Magdalena Birowska**

University of Warsaw, Poland  
Oral presentation

**Levan Chotorlishvili**

Rzeszów University of Technology, Poland  
Oral presentation

**Maciej Chrobak**

AGH University of Krakow, Poland  
Oral presentation

**Jakub Cwynar**

University of Warsaw, Poland  
Oral presentation

**Julia Czarnecka**

Leiden Probe Microscopy B.V., The Netherlands  
Oral presentation

**Semir El-Ahmar**

Poznań University of Technology, Poland  
Invited Speaker

**Karolina Filak-Mędoń**

Warsaw University of Technology, Poland  
Oral presentation

**Patryk Florczak**

Adam Mickiewicz University in Poznań, Poland  
Invited Speaker

**Costas Galiotis**

FORTH & University of Patras, Greece  
Plenary speaker

**Karol Gałązka**

University of Warsaw, Poland  
Poster presentation

**Mariusz Gołębiowski**

Maria Curie-Skłodowska University, Poland  
Poster presentation

**Luca Gregoratti**

Elettra Sincrotrone Trieste, Italy  
Invited Speaker

**Lukasz Grzegorzółka**

University of Warsaw, Poland  
Oral presentation

**Chris van Haesendonck**

KU Leuven, Belgium  
Invited Speaker

**Yumeng Hua**

West Pomeranian University of Technology, Poland  
Poster presentation

**Mirali Jafari**

Adam Mickiewicz University in Poznań, Poland  
Oral presentation

**Joanna Janusz**

Arctic Paper Kostrzyn SA  
Regular Participant

**Włodzimierz Jaskólski**

Nicolaus Copernicus University in Toruń, Poland  
Invited Speaker

**Paulina Jureczko**

University of Silesia, Poland  
Oral presentation

**Anna Kaczmarek**

Arctic Paper Kostrzyn SA  
Regular Participant

**Mikhail Katsnelson**

Radbound University Nijmegen, The Netherlands  
Plenary Speaker

**Tomasz Kędzierski**

West Pomeranian University of Technology, Poland  
Oral Presentation and poster presentation

**Aleksander Kolman**

Adam Mickiewicz University in Poznań, Poland  
Poster presentation

**Tomasz Kosmala**

University of Wrocław, Poland  
Invited Speaker

**Jan Kossacki**

University of Warsaw, Poland  
Oral presentation

**Piotr Kossacki**

University of Warsaw, Poland  
Invited Speaker

**Paweł J. Kowalczyk**

University of Łódź, Poland  
Invited Speaker

**Mariusz Krawiec**

Maria Curie-Skłodowska University, Poland  
Regular Participants

**Witold Krumplewski**

Adam Mickiewicz University in Poznań, Poland  
Poster presentation

**Marcin Kurpas**

University of Silesia in Katowice, Poland  
Oral presentation and poster presentation

**Grzegorz Leniec**

West Pomeranian University of Technology, Poland  
Oral presentation

**Aleksandra Leśniewicz**

Adam Mickiewicz University in Poznań, Poland  
Poster presentation

**Dorota Lewandowska**

Arctic Paper SA  
Regular Participant

**Sebastian Mackowski**

Nicolaus Copernicus University in Toruń, Poland  
Regular Participant

**Łukasz Majchrzycki**

Poznan University of Technology, Poland  
Oral presentation

**Jacek Majewski**

University of Warsaw, Poland  
Regular Participant

**Piotr Maksymiuk**

University of Warsaw, Poland  
Oral presentation

**Grzegorz Mariańczyk**

Arctic Paper SA  
Regular Participant

**Klaudia Maślana**

West Pomeranian University of Technology, Poland  
Oral presentation and poster presentation

**Lena Miler**

University of Warsaw, Poland  
Oral presentation

**Ireneusz Morawski**

University of Wrocław, Poland  
Oral presentation

**Aleksandra Nadolska**

University of Lodz, Poland  
Oral Presentation

**Justyna Olejnik**

Politechnika Wroclawska, Poland  
Poster presentation

**Marta Pelc**

Nicolaus Copernicus University in Toruń, Poland  
Oral presentation and poster presentation

**Karolina Pietruszewicz**

West Pomeranian University of Technology, Poland  
Oral presentation

**Piotr Pigoń**

AGH University of Krakow, Poland  
Oral presentation

**Przemysław Przybysz**

University of Lodz, Poland  
Oral presentation

**Piotr Radomski**

Poznan University of Technology, Poland  
Oral presentation and poster presentation

**Izabela Rogala**

University of Warsaw, Poland  
Oral presentation

**Maciej Rogala**

University of Lodz, Poland  
Regular Participant

**Wojciech Rudziński**

Adam Mickiewicz University in Poznań, Poland  
Oral presentation

**Adam Rycerz**

Jagiellonian University in Kraków, Poland  
Invited Speaker

**Paweł Sać**

West Pomeranian University of Technology, Poland  
Poster presentation

**Sanjay Sahare**

Adam Mickiewicz University in Poznań, Poland  
Oral presentation

**Anika Schlenhoff**

University of Münster, Germany  
Invited Speaker

**Viera Skákalová**

Slovak Academy of Sciences in Bratislava, Slovakia  
Invited Speaker

**Marina Smirnova**

Adam Mickiewicz University in Poznań, Poland  
Poster presentation

**Mykhailo Solovan**

Adam Mickiewicz University in Poznań, Poland  
Poster presentation

**Maciej Szary**

Poznan University of Technology, Poland  
Poster presentation

**Maciej Szyszko**

University of Warsaw, Poland  
Oral presentation

**Klaas-Jan Tielrooij**

Eindhoven University of Technology, The Netherlands  
Invited Speaker

**Klaudia Toczek**

University of Lodz, Poland  
Oral presentation

**Konrad Wilczyński**

Warsaw University of Technology, Poland  
Oral presentation

**Izabella Wojciechowska**

Adam Mickiewicz University in Poznań, Poland  
Oral presentation

**Paweł Wojciechowski**

Maria Curie-Skłodowska University, Poland  
Oral presentation

**Jolanta Woronowska**

West Pomeranian University of Technology, Poland  
Poster presentation

**Andrzej Wysmolek**

University of Warsaw, Poland  
Regular Participant

**Thomas Vasileiadis**

Adam Mickiewicz University in Poznań, Poland  
Invited Speaker

**Luca Vattuone**

University of Genoa, Italy  
Invited Speaker

**Qingshan Yang**

West Pomeranian University of Technology, Poland  
Poster presentation

**Mariusz Zdrojek**

Warsaw University of Technology, Poland  
Regular Participant

**Ryszard Zdyb**

Maria Curie-Skłodowska University, Poland  
Passive Participation

**Ewa Żuberek**

Wrocław University of Science and Technology, Poland  
Poster presentation