

7th Polish Conference
Graphene and other 2D materials



Abstract Book

Łódź, September 12th-14th, 2022



**FACULTY OF PHYSICS
AND APPLIED INFORMATICS**
University of Lodz

www.graphene2d.uni.lodz.pl

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Dear researchers, scientists, nanotechnologists,

We are pleased to invite you to participate in the latest edition of the conference on graphene and 2D materials. The 7th Polish Conference “Graphene and other 2D materials” will be held in Lodz, on September 12-14, 2022, at the University of Lodz.

The Faculty of Physics and Applied Informatics is responsible for the organization of the event.

The co-organizer of the conference is the Faculty of Physics of the University of Warsaw.

About the conference

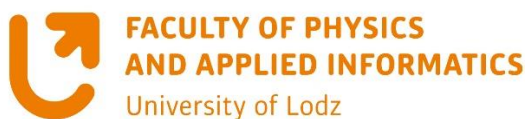
The aim of the conference is to present scientific results and exchange experiences as well as to consolidate the Polish and European scientific community related to nanoscience and nanotechnology, graphene materials and other 2D materials.

Previous editions were organized by the Wrocław University of Science and Technology (2021 - Online) and the West Pomeranian University of Technology in Szczecin.

The program includes both lectures by invited guests and presentations of selected works submitted to the Conference. A part of the submitted works will be presented during poster sessions. The official language of the conference is English.

The conference is addressed to a wide range of people involved in interdisciplinary research on the border of physics, chemistry and materials science. We warmly encourage both industry representatives and people starting their scientific careers to participate in the conference.

On behalf of the organizing committee, we wish every participant a pleasant and fruitful conference.



Partners

Technolutions
sp. z o. o.



COMEF



SYL & ANT
Instruments



SYGNIS s.a.



PIK Instruments
sp. z o. o.



BeeGraphene
sp. z o. o.



EC1 ŁÓDŹ



Conference programme

Invited speakers

Adam Babiński, Faculty of Physics, University of Warsaw

Two-dimensional Semiconductors in Magnetic Field – Experimental Opportunities in the European Magnetic Field Laboratory

Magdalena Birowska, Institute of Theoretical Physics, University of Warsaw

Magnetic fingerprints in electronic and optical studies of 2D magnetic crystals

Leszek Bryja, Institute of Physics, Wrocław University of Science and Technology

Optical properties and lattice dynamics of van der Waals heterostructures of transition metal chalcogenides

Madhurya Chandel, Faculty of Materials Science and Engineering, Warsaw University of Technology

A novel and reproducible approach for the synthesis of Mbene

Artur Ciesielski, Université de Strasbourg, CNRS, Institut de Science et d'Ingénierie

Supramoléculaires, Centre for Advanced Technologies, Adam Mickiewicz University

Two-dimensional materials as platform for water purification and sensing

Martin Gmitra, Department of Theoretical Physics and Astrophysics,

Pavol Jozef Šafárik University in Košice

Exchange and spin-orbit coupling proximity effects in graphene embedded in van der Waals heterostructures

Szymon Godlewski, Institute of Physics, Jagiellonian University

On-surface synthesis of higher acenes and nanographenes

Agnieszka Jastrzębska, Faculty of Materials Science and Engineering, Warsaw University of Technology

Novel and intriguing two-dimensional Mbenes

Maciej Molas, Faculty of Physics, University of Warsaw

Excitonic complexes in layered van der Waals materials

Barbara Piętka, Institute of Experimental Physics, Faculty of Physics, University of Warsaw

2D-perovskites in microcavities: strong light-matter coupling regime and polariton condensate

Agnieszka Stępnia-Dybala, Institute of Physics, M. Curie-Skłodowska University

Silicene formations on Pb-Si heterostructures

The schematic programme

Monday 12.09.2022		Tuesday 13.09.2022		Wednesday 14.09.2022	
9:15 - 9:35	Open	9:15 - 9:50	Birowska	9:15 - 9:50	Jastrzębska
9:35 - 10:10	Gmitra	9:50 - 10:25	Babiński	9:50 - 10:25	Chandel
10:10 - 10:25	Ludwiczak				
10:25 - 10:40	Wojciechowska	10:25 - 10:40	Kulka	10:25 - 10:40	Jakubczak
10:40 - 10:55	Kurpas	10:40 - 10:55	Szałowski	10:40 - 10:55	Purbayanto
10:55 - 11:25	<i>Coffee</i>	10:55 - 11:25	<i>Coffee</i>	10:55 - 11:25	<i>Coffee</i>
11:25 - 12:00	Godlewski	11:25 - 12:00	Ciesielski Artur	11:25 - 12:00	Stępnia-Dybala
12:00 - 12:15	Gołębiowski	12:00 - 12:15	Baranowska	12:00 - 12:15	Haniś
12:15 - 12:30	Olkowska-Pucko	12:15 - 12:30	Lewandowska-Andrałojć	12:15 - 12:30	Kierdaszuk
12:30 - 12:45	Iwański	12:30 - 12:45	Środa	12:30 - 12:45	Giza
12:45 - 13:00	Ciesielski Arkadiusz	12:45 - 13:00	Bury	12:45 - 13:00	Le Ster
13:00 - 14:30	<i>Lunch</i>	13:00 - 14:30	<i>Lunch</i>	13:00 - 13:10	Conference Closing
14:30 - 15:05	Bryja	14:30 - 15:05	Piętka	13:10 - 14:30	<i>Lunch</i>
15:05 - 15:20	Binder	15:05 - 15:20	Daniszewska		
15:20 - 15:35	Zawadzka	15:20 - 15:35	Ojrzyńska		
15:35 - 15:50	Wilczyński	15:35 - 15:50	Rogoża		
15:50 - 16:05	Czerniak-Łosiewicz	15:50 - 16:05	Comef		
16:05 - 16:35	<i>Coffee</i>	16:05 - 16:35	<i>Coffee</i>		
16:35 - 17:10	Molas				
17:10 - 17:25	Filak				
17:25 - 17:40	Kędzierski				
17:40 - 17:55	Pakulski				
17:55 - 18:05	Technolutions				
18:15 - 20:15	Poster session	18:45 - 19:45	<i>Guided tour of the revitalized EC1 Power Plant</i>		
		20:00 - 22:00	<i>Dinner EC1 Łódź</i>		

7th Polish Conference *Graphene and other 2D materials*, Lodz 2022

Monday, September 12th, 2022.

9:15 - 9:35	Open	
	Chair: Magdalena Birowska	
	Martin Gmitra	
9:35 - 10:10	M. Exchange and spin-orbit coupling proximity effects in graphene embedded in van der Waals heterostructures	
	Katarzyna Ludwiczak	
10:10 - 10:25	K. Proximity Effect of Two-dimensional Magnets on Hexagonal Boron Nitride: Optical Studies	
	Anita Wojciechowska	
10:25 - 10:40	Surface interactions of the 2D rare MXenes with organic macromolecules	
	Marcin Kurpas	
10:40 - 10:55	Proximity spin-orbit coupling in carbon nanotubes on 2D materials	
10:55 - 11:25	Coffee	
	Chair: Agnieszka Stępiak-Dybala	
	Szymon Godlewski	
11:25 - 12:00	On-surface synthesis of higher acenes and nanographenes	
	Mariusz Gołębiowski	
12:00 - 12:15	β phase of antimonene on W(110) – growth, morphology and crystallographic structure	
	Katarzyna Olkowska-Pucko	
12:15 - 12:30	Transition metal dichalcogenide alloys as a new class of materials	
	Jakub Iwański	
12:30 - 12:45	Temperature induced giant shift of phonon energy in epitaxial boron nitride layers	
	Arkadiusz Ciesielski	
12:45 - 13:00	Fabrication of Distributed Bragg Reflectors via MOCVD growth of porous BN layers with high refractive index contrast	
13:00 - 14:30	Lunch	
	Chair: Joanna Jadczyk	
	Leszek Bryja	
14:30 - 15:05	Optical properties and lattice dynamics of van der Waals heterostructures of transition metal chalcogenides	
	Johannes Binder	
15:05 - 15:20	Raman optical activity of 1T-TaS ₂	
	Natalia Zawadzka	
15:20 - 15:35	Defect-related emission of HfS ₂	
	Konrad Wilczyński	
15:35 - 15:50	First principles and Raman investigation of phonon anharmonicity and thermal expansion in 1-5-layered WS ₂ nanosheets	
	Karolina Czerniak-Łosiewicz	
15:50 - 16:05	Unraveling the Mechanism of the Large Photocurrent Enhancement in 2D Transition Metal Dichalcogenides by Plasma Treatment	
16:05 - 16:35	Coffee	
	Chair: Leszek Bryja	
	Maciej Molas	
16:35 - 17:10	Excitonic complexes in layered van der Waals materials	
	Karolina Filak	
17:10 - 17:25	FEP/graphene nanocomposites for multipurpose applications	
	Tomasz Kędzierski	
17:25 - 17:40	Thin films composed of expanded reduced graphene oxide and exfoliated WS ₂ as anode materials in Li-ion batteries	
	Dawid Pakulski	
17:40 - 17:55	Metal Organic Polymers as high-capacity energy storage material	
17:55 - 18:05	Company presentation: Technolutions	
	Pause	
18:15 - 20:15	Poster session	

7th Polish Conference *Graphene and other 2D materials*, Lodz 2022

Tuesday, September 13th, 2022.

<i>Chair: Agnieszka Jastrzębska</i>	
9:15 - 9:50	Magdalena Birowska <i>Magnetic fingerprints in electronic and optical studies of 2D magnetic crystals</i>
9:50 - 10:25	Adam Babiński <i>Two-dimensional Semiconductors in Magnetic Field –Experimental Opportunities in the European Magnetic Field Laboratory</i>
10:25 - 10:40	Teresa Kulka <i>Magnetic properties of Ti₂C MXenes doped with transition metals Cr, Mn, and Fe</i>
10:40 - 10:55	Karol Szałowski <i>Electric field-controlled spin state in urethane-like nanographenes: computational study</i>
10:55 - 11:25	<i>Coffee</i>
<i>Chair: Maciej Molas</i>	
11:25 - 12:00	Artur Ciesielski <i>Two-dimensional materials as platform for water purification and sensing</i>
12:00 - 12:15	Daria Baranowska <i>Nanowired g-C₃N₄ for H₂ photogeneration from water splitting</i>
12:15 - 12:30	Anna Lewandowska-Andrałojć <i>Functionalization of Ti₃C₂T_x with dyes: spectroscopic insights and photocatalytic applications</i>
12:30 - 12:45	Bartosz Środa <i>ZIF-67/MXene composites as a highly efficient electrocatalyst for oxygen evolution reaction</i>
12:45 - 13:00	Dominika Bury <i>On the photocatalytic activity of the oxidation stabilized Ti₃C₂T_x MXene</i>
13:00 - 14:30	<i>Lunch</i>
<i>Chair: Andrzej Wyszomłek</i>	
14:30 - 15:05	Barbara Piętka <i>2D-perovskites in microcavities: strong light-matter coupling regime and polariton condensate</i>
15:05 - 15:20	Agata Daniszewska <i>Technology of graphene flakes production via liquid phase exfoliation and their properties characterization</i>
15:20 - 15:35	Milena Ojrzyńska <i>Production of graphene flakes based on combined SO₃ intercalation-exfoliation method</i>
15:35 - 15:50	Jakub Rogoża <i>Metallic contacts and processing of epitaxial boron nitride</i>
15:50 - 16:05	Company presentation: Comef
16:05 - 16:35	<i>Coffee</i>
	Pause
18:45 - 19:45	<i>Guided tour of the revitalized EC1 Power Plant</i>
20:00 – 22:00	<i>Dinner EC1 Łódź</i>

Wednesday, September 14th, 2022

<i>Chair: Adam Babiński</i>	
9:15 - 9:50	Agnieszka Jastrzębska <i>Novel and intriguing two-dimensional MBenes</i>
9:50 - 10:25	Madhurya Chandel <i>A novel and reproducible approach for the synthesis of MBene</i>
10:25 - 10:40	Michał Jakubczak <i>Nb-MXenes bioremediation with green microalgae: The mechanism of action and a road to decomposition</i>
10:40 - 10:55	Muhammad Purbayanto <i>Tunable Antibacterial Activity of a Polypropylene Fabric Coated with Bristling Ti₃C₂T_x MXene Flakes Coupling the Nanoblade Effect with ROS Generation</i>
10:55 - 11:25	<i>Coffee</i>
<i>Chair: Martin Gmitra</i>	
11:25 - 12:00	Agnieszka Stępniań-Dybala <i>Silicene formations on Pb-Si heterostructures</i>
12:00 - 12:15	Jozef Haniš <i>Quasiparticle Interference in Superconducting Layered Misfit Compounds (LaSe)_{1.14}(NbSe₂)_x, x=1,2.</i>
12:15 - 12:30	Jakub Kierdaszuk <i>Gating and electrostatically-induced strain of graphene on nanorods</i>
12:30 - 12:45	Małgorzata Giza <i>Influence of 2-dimensional interlayers on contact resistance in TMDs-based field-effect transistors</i>
12:45 - 13:00	Maxime Le Ster <i>Moiré superlattices in reciprocal space</i>
13:00 - 13:10	Conference closing
13:10 - 14:30	<i>Lunch</i>

Monday
September 12th, 2022

The detailed programme

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17:55 - 18:05	Company presentation: Technolutions
	Pause
18:15 - 20:15	Poster session

Exchange and spin-orbit coupling proximity effects in graphene embedded in van der Waals heterostructures

M. Gmitra^{1,2}

¹ *Institute of Physics, Pavol Jozef Šafárik University in Košice, Park Angelinum 9, 040 01 Košice, Slovakia*

² *Institute of Experimental Physics, Slovak Academy of Sciences, Watsonova 47, 040 01 Košice, Slovakia*

Bare electronic structure of graphene limits its applications due to lack of magnetic order and weak spin-orbit coupling. Embedding it in van der Waals heterostructures [1] opens new venues for utilizing induced proximity effects [2] in novel device design [3]. In the talk we discuss induced spin-orbit coupling and exchange coupling proximity effects in graphene [4] and bilayer graphene [5] on transition metal dichalcogenides and on two dimensional magnets [6] and twisting effects [7]. Specially we analyze 1T-TaS₂ which undergoes charge density wave and spontaneous magnetic transition at low temperatures. The proximity effects on electronic states in graphene near the Dirac point will be discussed in terms of density functional theory and an effective tight-binding model. An emphasis will be given to extracted model parameters relevant for realistic modeling of low energy electronic structure of graphene.

Acknowledgments: This work was supported by the project APVV SK-PL-21-0055, VEGA Grant No. 1/0105/20, Slovak Academy of Sciences project IMPULZ IM-2021-42 and project FLAG ERA JTC 2021 2DSOTECH.

- [1] A.K. Geim, I.V. Grigorieva, *Nature* **499**, 419-425 (2013).
- [2] I. Žutić, A. Matos-Abiague, B. Scharf, et al. *Materials Today* **22**, 85-107 (2019).
- [3] W. Han, R.K. Kawakami, M. Gmitra, et al. *Nature Nanotechnology* **9**, 794-807 (2014).
- [4] M. Gmitra, J. Fabian, *Phys. Rev. B* **92**, 155403 (2015).
- [5] M. Gmitra, J. Fabian, *Phys. Rev. Lett.* **119**, 146401 (2017).
- [6] K. Zollner, M. Gmitra, J. Fabian, *Phys. Rev. Lett.* **125**, 196402 (2020).
- [7] T. Naimer, K. Zollner, M. Gmitra, et al. *Phys. Rev. B* **104**, 195156 (2021).

Proximity Effect of Two-dimensional Magnets on Hexagonal Boron Nitride: Optical Studies

K. Ludwiczak¹, J. Binder¹, A.K. Dąbrowska¹, J. Sitnicka¹, J. Jasiński², R. Stępniewski¹,
A. Wyszomółka¹

¹ University of Warsaw, Pasteura 5, 02-093 Warsaw, Poland

² University of Louisville, 2301 S 3rd St, Louisville, KY 40292, United States of America

Hexagonal boron nitride (hBN) is a wide bandgap material (~ 6 eV) commonly used in the study of other 2D crystals as a substrate or an insulator in heterostructures. The material itself provides a great platform to study basic physical phenomena, especially after the discovery of single photon emission (SPE) from its defects [1].

While the exact mechanism of the emission and the nature of the responsible defects are still being discussed, recent studies [2,3] show that the emission from hBN can be altered by an external magnetic field.

In this work, we study the proximity effect between hBN and two-dimensional magnets from the chromium halides family. Our approach allows to address paramagnetic centers in hBN locally, which stands as an intriguing alternative to externally applied magnetic fields. We studied the optical response of hBN/CrBr₃/hBN heterostructures and found an additional peak in the photoluminescence spectrum at low (liquid helium) temperature correlated with the magnetic ordering in CrBr₃ (Fig 1).

Our work constitutes a step towards understanding the quantum emission from defects in hBN and may lead to finding new applications of this material, for instance in the field of quantum information technology.

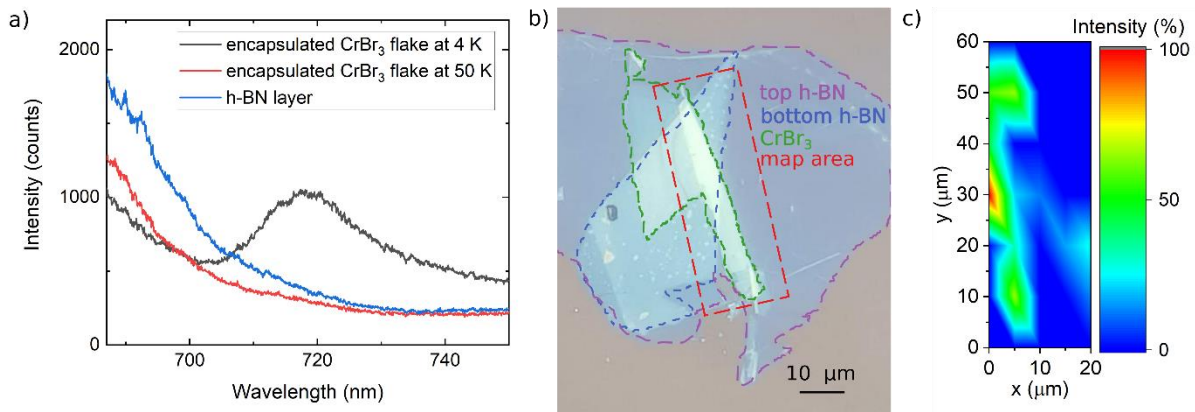


Fig. 1. a) Photoluminescence spectra of a hBN/CrBr₃/hBN heterostructure. b) Optical microscope image of the studied heterostructure. c) Intensity map of the additional photoluminescence peak of the studied heterostructure.

Acknowledgments: This work is supported by National Science Centre, Poland under the decision 2021/41/N/ST3/03579

[1] T. Tran, *et al.*, Nature Nanotechnology **11**, 37 (2016).

[2] A. L. Exarhos, *et al.* Nature Communications **10**, 222 (2019).

[3] M. Koperski, *et al.* Optics Communications **411**, 158 (2018).

Surface interactions of the 2D rare MXenes with organic macromolecules

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² *Department of Physics and Engineering Physics, Tulane University,
New Orleans, LA 70118, USA*

MXenes are a new class of 2D materials. Their name reflects their stoichiometry $M_{n+1}X_n$, where M denotes a transition metal and X stands for carbon or nitrogen. They are obtained by the selective etching of the A atom from the MAX phases.

Since the discovery of the MXenes phases in 2011 to the present day, many publications have appeared that mainly concern the properties of the MXenes phases from the Ti-C system. In this paper, we will present an in-depth study of the colloidal properties of the rare MXenes phases such as Nb₂C and Nb₄C₃. We will also present a comprehensive study of changes in the surface properties of the rare MXenes phases under the influence of interactions with cationic proteins - lysozyme and collagen. The research will be carried out using the method of dynamic light scattering and zeta potential. The aim of this experiment is to find out how the structure, surface chemistry and concentration of a bio-macromolecules affect the interaction of MXenes with collagen and lysozyme.

Acknowledgments: The study was accomplished thanks to the funds allotted by the National Science Centre, Poland, within the framework of the research projects 'PRELUDIUM 17' no. UMO-2019/33/N/ST5/02095 and 'SONATA BIS 7' no. UMO-2017/26/E/ST8/01073.

Proximity spin-orbit coupling in carbon nanotubes on 2D materials

M. Kurpas¹

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We employ first principles calculations based on the density functional theory and study proximity spin-orbit effects in heterostructures made of a 1D carbon nanotube and a 2D material. We find, that in contrast to periodic 2D systems, in which the crystal potential across the interface is rather smooth, in 1D/2D heterostructures it displays a substantial in-plane variation due to the finite size of the nanotube. This leads to the emergence of new types of effective spin-orbit fields absent in 2D systems [1]. In effect, the Dirac cone bands of the nanotube split off in a similar way as in the case coexisting external electric and magnetic fields [2]. Our results show that proximized carbon nanotubes can realize interesting physical phenomena, such as helical modes, and are promising systems for spintronics applications.

Acknowledgments: Work supported by the V4-Japan Joint Research Program on Advanced Materials “BgapEng” (DWM/V4-JAPAN/2/431/2021).

[1] M. Kurpas, in preparation.

[2] J. Klinovaja et al. Phys. Rev. B **84**, 085452 (2011).

On-surface synthesis of higher acenes and nanographenes

S. Godlewski¹

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In recent years we observe renewed interest in the development of electronics based on electron transport through single molecules. Among different families of organic species, acenes and nanographenes hold the special position. In particular a lot of effort is undertaken to achieve efficient synthetic strategies to generate such well-defined sections of graphene or graphene-like modules with diverse topological modifications. However, the reactivity/instability of numerous molecules as well as the insolubility of large polycyclic aromatic hydrocarbons limits the applications of conventional chemistry methods. An attractive alternative to the solution chemistry is based on its combination with the on-surface synthesis approach.

Acenes are attracting considerable interest due to the intriguing electronic properties originating from only one Clar π -sextet regardless of the molecule length. However, the unique π -electron system causes the molecules to be more reactive and less stable with increased number of annulated rings. Consequently, this makes their synthesis, detailed characterization and functionalization a very challenging task. In recent years some successful strategies toward fabrication of higher acenes and their derivatives have been reported, e.g., some long acenes were stabilized and detected within noble gas matrices or in polymers. However, only recently the on-surface chemistry approach allowed for synthesis and characterization of higher acenes.

Herein we present the on-surface generation of higher acenes [1-2], their analogues [3] and diverse nanographenes [4-5], as well as the detailed study of their electronic structure on the Au(111) surface. Our method is based on the two-step dehydrogenation and thermally induced sequential cyclodehydrogenation of a stable and easily handled molecular precursors.

High-resolution non-contact atomic force microscopy (NC-AFM) imaging was applied for the detailed visualization of the internal structure of the intermediates, as well as the target molecules with diverse topologies. Details on the electronic structure were revealed using high resolution dI/dV mapping.

The research was supported by the National Science Center, Poland (2017/26/E/ST3/00855).

- [1] R. Zuzak, et al., *ACS Nano* **11**, 9321–9329 (2017).
- [2] R. Zuzak, et al., *Angew. Chem. Int.Ed.* **57**, 10500–10505 (2018).
- [3] I. Izydorczyk, et al., *Angew. Chem. Commun.* **58**, 4063 – 4066 (2022).
- [4] R. Zuzak, et al., *Chem. Commun.* **54**, 10256-10259 (2018).
- [5] R. Zuzak, et al., *Chem. Sci.* **10**, 10143-10148 (2019).

β phase of antimonene on W(110) – growth, morphology and crystallographic structure

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Antimonene is a novel two-dimensional material which consists of two sublattices of antimony atoms. Theoretical calculations predict a number of antimonene allotropes among which only α and β phases have been obtained in experiments. The former phase has rectangular crystallographic structure, while the latter one has honeycomb structure. Antimonene exhibits unique properties – tunable energy band gap, possibility of transition from indirect to direct band gap and very low thermal conductivity, to name a few [1]. Up to now, epitaxial growth of antimonene was successfully realized on substrates like SiO₂, PbTe₂, Ge(111), Ag(111), Cu(111) and Cu(110) [2]. Here, we report on the formation of β -antimonene on W(110).

Spin polarized low energy electron microscope (SPLEEM) has been used during synthesis and investigations of the β phase of antimonene. The microscope works under ultrahigh vacuum conditions with the base pressure of $3 \cdot 10^{-11}$ mbar. The main chamber of microscope is equipped with effusion cells which enable preparation of samples by epitaxial growth method. To observe surface topography and diffraction patterns of the prepared samples the LEEM and LEED modes have been used, respectively.

During the epitaxial growth of Sb layers on W(110) mainly α phase of antimonene was observed. However, in some regions one can identify creation of another allotrope. LEED investigations proved that this allotrope has honeycomb arrangement of atoms corresponding to the β phase of antimonene. The lattice constant of 4.03 Å of this structure is in excellent agreement with the reported experimental results: 4.09 Å [3] and 4.13 Å [4]. It appears that the β -antimonene is formed on the two-domain α -antimonene layer. It results in the formation of 4 domains of the β phase rotated by 15° relative to each other. The morphology of the β -antimonene layer reflects the arrangement of the Sb atoms in the honeycomb structure identified in the diffraction patterns. The preparation procedure of these two dimensional materials needs further optimization, however, it already seems to be very promising for making β -antimonene in the macroscopic scale.

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Transition metal dichalcogenide alloys as a new class of materials

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Monolayers (MLs) of semiconducting transition metal dichalcogenides (S-TMDs), e.g., MoSe₂ and WSe₂, are direct bandgap semiconductors characterized by very interesting optical and electronic properties. Alloys of S-TMDs have emerged as materials with tunable electronic structures and valley polarizations [1]. It is therefore crucial to uncover their basic optical properties.

To this end we investigate the low-temperature magneto-photoluminescence (PL) of Mo_{0.5}W_{0.5}Se₂ ML embedded in hexagonal boron nitride (hBN) flakes. Measurements were done in magnetic field up to 30 T applied in two configurations: out-of-plane and in-plane. The MoWSe₂ ML should combine the properties of both “parents”, which are members of different ML families. The WSe₂ MLs belong to the so called “darkish” MLs, in which the excitonic ground state is optically inactive (dark), while the MoSe₂ MLs is a representative of “bright” MLs with optically active ground state [2]. The zero-field low-temperature PL spectra spectrum is composed of two well resolved emission lines, denoted as X and T, which we attribute correspondingly to the neutral and charged excitons. Upon application of the out-of-plane magnetic field, these transitions split into two circularly polarized components (σ^{\pm}) due to the excitonic Zeeman effect. We extracted transition energies, and, on this basis, we determined effective Lande g-factors. It is seen that the g-factors for both transitions significantly differ. While the g-factor of the T line of about -4.7 is similar to the reported value of about -4 [3], the g-factor of the X line is much bigger and equal to -7.3. Using DFT calculations, we predict that this value can be understood in terms of particular arrangements of bands in the investigated Mo_{0.5}W_{0.5}Se₂ ML. Moreover, the application of the in-plane magnetic field to the ML reveals an additional line observed in magnetic fields above 25 T. This transition is apparent around 16 meV below the X line. We show how our results support the conclusion that the Mo_{0.5}W_{0.5}Se₂ ML is a “darkish” material with bright dark exciton splitting very similar to that of the MoS₂ ML [4].

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Temperature induced giant shift of phonon energy in epitaxial boron nitride layers

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Hexagonal boron nitride (hBN) as an atomically flat, two-dimensional insulator, appears in many novel applications (e.g., van der Waals heterostructures). However, most of the applications are based on small flakes exfoliated from the bulk crystal. In many cases, it is an obstacle which hinders the introduction of hBN in large-scale applications. One possible solution for this problem is epitaxial growth that permits to obtain few-inch area layers [1]. However, the structural and optical quality of the epitaxial layer is still inferior to flakes exfoliated from the bulk crystal [2]. Improving the quality of epitaxial layers requires a deeper understanding of the defect properties and their mechanisms of creation.

In this work we present temperature-dependent (160-540 K) Fourier-transform infrared spectroscopy (FTIR) studies of the E_{1u} phonon of boron nitride epitaxial layers grown with Metal Organic Vapor Phase Epitaxy (MOVPE). Comparing results obtained for as-grown and delaminated layers [3], we reveal a significant reduction of the layer-substrate interaction for as-grown samples, which is caused by wrinkles formation during cooling down the material after the growth process. This result is of particular importance regarding the aspect of combining epitaxial boron nitride layers with other materials. However, the most striking result emerging from our studies is a giant, anomalous shift of phonon energy in a narrow temperature range. The temperature for which the anomaly occurs is sensitive to heating, cooling and UV light irradiation. We present a model involving a temperature-induced charge redistribution leading to changes of the charge state of certain defects. This in turn causes compressive strain in the epitaxial layer, that would have to be of the order 0.1 % [4] to explain the observed shift. The narrow temperature range in which the anomalous behaviour takes place raises the question of an involvement of pyro- and piezoelectric effects, which can be expected for non-centrosymmetric stackings of BN monolayers. The issue of the properties of different sp^2 -BN stacking is very timely and is of rising interest among scientists [5].

Acknowledgment: This work was supported by the National Science Centre, Poland, under decisions 2019/33/B/ST5/02766 and 2020/39/D/ST7/02811.

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Fabrication of Distributed Bragg Reflectors via MOCVD growth of porous BN layers with high refractive index contrast

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Distributed Bragg Reflectors (DBRs) are commonly used in photonic devices such as Vertical Cavity Surface Emitting Lasers (VCSELs) or Resonant Cavity Light Emitting Diodes (RCLEDs). DBRs are multi-layered structures, in which layers with high and low values of refractive index are deposited alternately on top of each other in a form of a superlattice. As a result of interference of multiple reflected beams, for a certain wavelength range, the normal reflectance approaches 100% [1]. Utilizing Metal-Organic Chemical Vapor Deposition (MOCVD) to fabricate DBR structures is already established. However, boron-based materials have not been considered for this purpose until recently [2,3]. Typically, the refractive index contrast is achieved by using two different materials, however it can also be achieved when at least one component layer is porous [4].

In this communication, we discuss the fabrication as well optical and structural characterization of porous Boron Nitride (BN) layers using the MOCVD. We show, that by manipulating the growth parameters, we are able to fabricate BN films with varying degrees of porosity, tuning the refractive index values of the acquired layers. We also show that two types of BN layers with different porosity can be deposited on top of each other multiple times, creating a DBR in a single growth process. For DBR structures consisting of 15.5-layer pairs, we were able to achieve a peak reflectance close to 90% [5]. Moreover, we were also able to construct a tunable optical microcavity based on the fabricated DBRs. Other kinds of applications will also be discussed.

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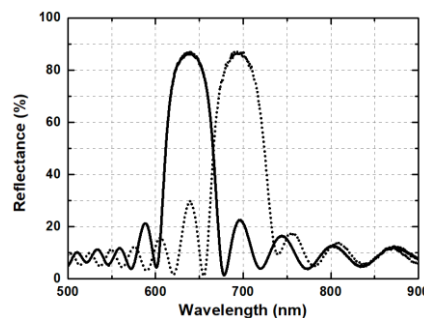


Fig. 1. Reflectance curves of two sample DBRs – with layer thickness optimized for 635 nm (continuous curve) and 693 nm (dotted curve)

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Optical properties and lattice dynamics of van der Waals heterostructures of transition metal chalcogenides

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The semiconducting monolayer transition metal dichalcogenides (TMDs) emerge as a unique platform to study electron- electron and electron- phonon interaction. Due to weak van der Waals bonds between the atomic layers in TMDs and hexagonal boron nitride (hBN) they can easily be assembled into so called van der Waals (vdW) heterostructures which exhibit much higher quality than TMDs monolayers exfoliated directly on SiO₂/Si substrates. The monolayer TMDs host variety of intra- and inter- valley neutral and charged excitonic complexes, which are either optically active or inactive due to the conservation of a spin or a momentum. Here, I will present results of optical studies of vdW heterostructures TMDs, composed of hBN flakes and monolayers of MoS₂, MoSe₂, WS₂, and WSe₂. First, I will focus on variety of excitonic complexes observed in low temperature PL spectra of W-based monolayers, which are positioned energetically below the bright direct exciton. Then, I will present how momentum-forbidden dark excitons reveal in photoluminescence up-conversion spectra of W-based vdW structures [1].

Additionally, I will discuss efficient room temperature multi-phonon upconversion of photoemission in monolayer semiconductor WS₂ [2]. I will also discuss the fine trion structure in monolayer MoS₂ [3]. In addition to interlayer electron-electron interactions, the interlayer electron-phonon coupling has a strong impact on the physical properties of the van der Waals heterostructures. Hence, in the second part of my talk I will focus on presentation both a strong increase in the emission intensity as well as a preservation of the helicity of the excitation light in the emission from vdW hBN/WSe₂/hBN heterostructures related to interlayer electron-phonon coupling [4].

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Raman optical activity of 1T-TaS₂

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Tantalum disulfide (TaS₂) belongs to the intensively studied family of layered transition metal dichalcogenides (TMDCs). The 1T polytype is an intriguing material, featuring numerous astonishing properties: it has temperature-dependent charge density wave phase transitions accompanied by periodic lattice distortions.

Raman spectroscopy is a relatively fast and non-invasive technique, widely used to study two-dimensional crystals. In case of 1T-TaS₂ it is a very convenient tool to investigate phase transitions. The remarkably rich structure of low-temperature Raman spectra is associated with a metal-insulator transition, which is accompanied by crystal lattice reorganization and formation of a new unit cell.

In this work, we present full angular polarization dependencies of the Raman modes of

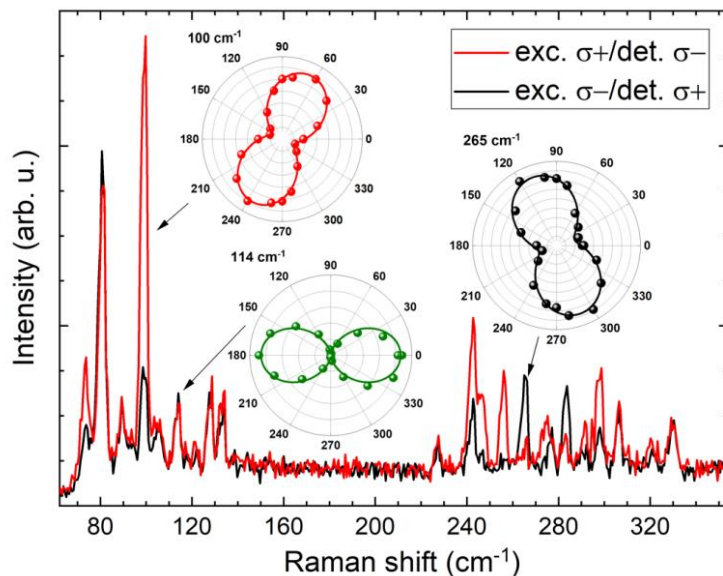


Fig. 1: Raman spectra excited by circularly polarized light. The differences in the spectra in the σ^+/σ^- and σ^-/σ^+ configurations are a sign of Raman optical activity. The insets show the corresponding angular plots of linear polarization for three classes of lines, which remain either unaltered or show an increase (decrease) in intensity [2].

confirmed recently [3]. Our results suggest that ROA may be used as a universal tool to study chiral properties of quantum materials.

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Defect-related emission of HfS₂

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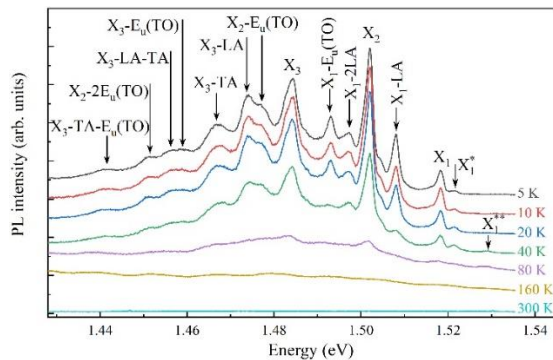
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Semiconductor transition metal dichalcogenides (TMDs), which are layered van der Waals (vdW) materials have emerged as fascinating objects to explore novel excitonic phenomena. The main focus of researchers has been focused until now on Mo- and W-based compounds. Recently however, hafnium based TMDs (i.e., HfS₂ and HfSe₂), have drawn more attention due to their very effective electrical response. This justifies a need to uncover their basic optical and electrical properties [1]. We report an optical emission from HfS₂ bulk crystal grown by chemical vapor transport method. The photoluminescence (PL) is investigated in a broad range of temperature (5-300 K).

The low-temperature emission consists of a series of well-resolved emission lines apparent in the energy range of 1.3-1.5 eV (see Figure). Three zero-phonon emission lines denoted as X₁, X₂, and X₃ can be distinguished, which are accompanied by their phonon replicas. The replicas with several optical and acoustic phonons can be identified as it is shown in the Figure. Moreover, the high-energy satellites of the X₁ line gain in their relative intensity with increasing temperature.



We attribute the observed emission to the recombination of bound excitons in HfS₂. It is proposed that these are neutral iodine molecules I₂, intercalated in vdW gaps between covalently bonded HfS₂ layers, which introduce to the material the potential localizing excitons. The I₂ molecules are introduced into the crystal during growth as iodine is used as a transport agent in the growth process. Similar low-temperature PL, related to intercalated halogen

molecules was previously observed in 2H polytypes of tungsten sulphides/selenides: WSe₂:I₂ [2] or WS₂:I₂ [2]. The ability of TMDs to serve as hosts to intercalating molecules originates from their vdW gaps. The space localization of such exciton leads to their delocalization in the momentum space. The exciton can therefore couple to phonons from a whole Brillouine zone. This explains the presence in the spectra the replicas at the energies corresponding to maxima of the total density of phonon states in bulk HfS₂, rather than energies of phonons from particular high-symmetry points of the Brillouin zone. The presence of iodine in the investigated samples is confirmed by secondary ion mass spectroscopy, which supports our attribution.

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First principles and Raman investigation of phonon anharmonicity and thermal expansion in 1-5-layered WS₂ nanosheets

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In this work, we study phonon anharmonicity in 1-5-layered WS₂ nanosheets, which is a representative example among transition metal dichalcogenides (TMDs) [1]. Anharmonicity has an important influence on the temperature-dependent phonon properties such as frequency and lifetime. For a substrate-supported sample, its lattice dynamics is further affected. Raman studies including the temperature-dependence [2] and substrate-induced effects (strain and doping) [3] were reported for the most popular TMDs such as MoS₂, also including few-layered films. However, a comprehensive DFT study of supported TMD films as a function of number of layers is missing in the literature.

Here, we present DFT and Raman study of temperature-dependent frequencies (Fig. 1) and bandwidths of the main Γ -point E_{2g}¹ and A_{1g} phonon modes in 1-5-layered WS₂ films. In the models, we include three-phonon interaction processes and thermal expansion. We obtain a very good consistency between simulated and experimental temperature trends (with respect to additive, temperature-independent corrections). Moreover, we simulate the impact of the substrate on phonon frequencies – including strain and charge doping. The presented study is significant due to the essential impact of phonon propagation on thermal and electrical transport in nanosheets – crucial for practical applications.

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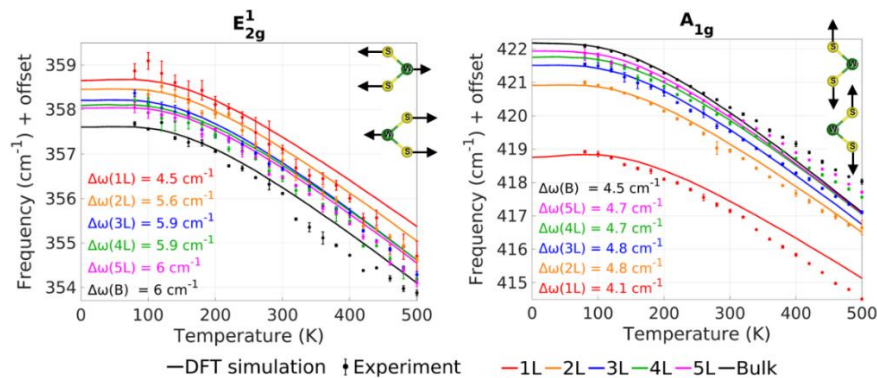


Fig. 1. DFT and Raman temperature-dependent frequencies of the E_{2g}¹ and A_{1g} phonon modes in 1-5-layered and bulk WS₂ [4]. The DFT results are shifted by constants (depicted in the figure).

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Unraveling the Mechanism of the Large Photocurrent Enhancement in 2D Transition Metal Dichalcogenides by Plasma Treatment

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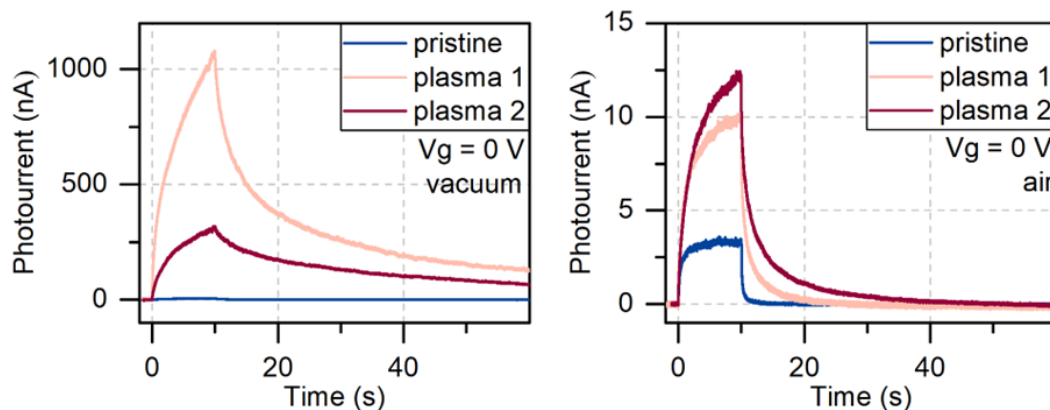
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Due to their favorable optoelectronic properties, transition metal dichalcogenides (TMDs) monolayers have been widely investigated to be used in optoelectronic applications ranging from photodetectors [1] to optical memories [2] and artificial optical synapses [3]. Different TMDs applications require different features such as fast response times and immediate relaxation for the detection or strong persistent photoconductivity for information storage. These contradictory features could be obtained by modifying the layers specifically for a given application, and the structural and chemical modifications should be studied to realize the applicational potential of 2D TMDs.

In this communication, we report an on-chip photocurrent modulation of MoS₂ and WS₂ monolayers by gentle plasma treatment. We obtain a significant enhancement in the photocurrent that shows the dependence on the measurement environment (vacuum or air). This environmental dependence allows us to attribute photocurrent enhancement to different mechanisms of the applied modification. We also note that apart from a large increase of the photocurrent, surface modification via plasma treatment is responsible for a slower response time of the layers.

This study shows how structural and chemical modification can be used to control the performance of the optoelectronic devices based on TMDs and tune the photoresponse to meet the needs of the specific optoelectronic applications.

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Excitonic complexes in layered van der Waals materials

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Atomically thin layers of semiconducting transition metal dichalcogenides (S-TMDs) MX_2 , where $\text{M} = \text{Mo}, \text{W}, \text{Re}, \text{Hf}, \text{etc.}$ and $\text{X} = \text{S}, \text{Se}, \text{or Te}$, represent a new class of materials, which are of vivid interest, primary in the area of semiconductor physics and nanoscience, as well as optoelectronic applications. The studies of thin films of S-TMDs are greatly inspired by and profit from the research and developments focused on graphene-based systems.

In my talk, I will give a concise overview of excitonic complexes apparent in S-TMDs. Particularly, the differences between “*bright*” and “*darkish*” MLs of Mo- and W-based S-TMDs will be discussed in terms of optical transitions. I will demonstrate that, in S-TMD MLs the *s*-type Rydberg series of excitonic states follows a simple energy ladder: $\epsilon_{nS} = -Ry^*/(n + \delta)^2$. The effective Rydberg energy in the formula, Ry^* is very close to the Rydberg energy scaled by the dielectric constant of the medium surrounding the ML and by the reduced effective electron-hole mass, whereas the ML polarizability is accounted for only by δ .

The second part of my talk will be devoted to the study of emission lines apparent in the low-temperature photoluminescence (PL) spectra of *n*-doped WS_2 ML embedded in hexagonal BN layers. Results of measurements in external magnetic fields and first-principles calculations will be reviewed. It will be demonstrated that apart from the neutral exciton line, all observed emission lines are related to the negatively charged excitons. Consequently, emissions due to both the bright (singlet and triplet) and dark (spin- and momentum-forbidden) negative trions as well as the phonon replicas of the latter optically inactive complexes are identified. The semidark trions and negative biexcitons are also distinguished. On the basis of their experimentally extracted and theoretically calculated *g*-factors, three distinct families of emissions are identified due to exciton complexes in WS_2 : bright, intravalley-, and intervalley-dark. The *g*-factors of the spin-split subbands in both the conduction and valence bands are also determined.

The last part of my presentation will be dedicated to the investigation of optical properties of a less known S-TMD, *i.e.*, ReSe_2 . It will be presented that the low-temperature PL spectra of anisotropic ReSe_2 layers display two linearly polarized emission lines, which blueshift by about 120 meV when the layer thickness decreases from 9 MLs to a monolayer.

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FEP/graphene nanocomposites for multipurpose applications

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Designing multipurpose material is an essential issue concerning solving problems with overweight modern electronics systems or their overheating or electromagnetic signal interference. Offering several properties in one product can significantly contribute to solving mentioned critical cases.

Within this work, we took on the production of such multipurpose material, which polymer nanocomposite was chosen.

In our specific case, the polymer matrix was fluorinated ethylene-propylene (FEP) with graphene nanoplatelets (GNP) as a filler. FEP is a high-temperature semicrystalline thermoplastic with favourable properties including high thermal stability, flammability, chemical resistance, dielectric strength, low water absorption and low melt viscosity [1]. Graphene nanoplatelets have unique well-known properties, what make their very promising in polymer nanocomposites application as a filler [2].

Different concentrations of GNP were dispersed in polymer matrix using mechanical mixer to obtain a well-homogenized mixture of particles and then hot-pressed in a hydraulic hot press. Electrical, thermal conductivity and electromagnetic interference (EMI) shielding efficiency of the composites have been investigated. The addition of a filler in the composite matrix enhances the mechanical properties of the material and improves its electrical and thermal conductivity. The excellent shielding efficiency of the composite has been proven in the X-band (8-12 GHz) region. Prepared graphene-based composites were significantly affected the dynamic mechanical characteristics such as storage, loss modulus, and damping factor. The presented FEP/GNP composites aim to develop a novel, low cost, light weight material with a great potential to be used for example as an efficient EMI shielding materials for electronic devices.

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Thin films composed of expanded reduced graphene oxide and exfoliated WS₂ as anode materials in Li-ion batteries

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With growing awareness of petrol and fossil fuels destructive impact on the environment, now more than ever the world needs an alternative route for obtaining electrical energy. Their most prominent successor are rechargeable lithium-ion batteries (LIBs), due to lithium low reduction potential (-3.04 V vs. SHE) and its over-the-top theoretical capacity (3860 mAh/g). The working electrode (or an anode) used commercially is graphite. In batteries, graphite is defined by its excellent stability, however its capacity is rather low (372 mAh/g). That is why researchers around the world are working constantly on new anode materials for LIBs. Examples of such materials are transition metal dichalcogenides (TMDs). They possess layered structure and are known to bond lithium ions. Unfortunately, these materials suffer from irreversible structure changes during charge/discharge process followed by deterioration of their electrochemical stability and capacity. This disadvantage, however, may be reduced by combining TMD with graphite derivative, like graphene oxide (GO). GO flakes tend to stick to one another, forming stable thin structures, called free-standing films. Additionally, terminated oxygen-rich groups increase the reactivity of graphene, allowing it to bond with other materials. Still, once oxidated, graphene loses its conductive properties. Yet, they can be restored after the reduction of GO, when reduced graphene oxide (rGO) is formed. Typical thermal route of reducing GO is to heat it in a furnace to very high temperatures. However, in 2020 a new way of reducing GO was established, by Chen *et al* [1]. They nicknamed this reaction Ultrafast and Self Expansion Reduction, or USER reaction. The reduction of GO to rGO transpired thanks to the rapid disintegration and elimination of oxygen-rich functional groups in graphene oxide. When film is quickly heated carbon oxides leave its structure and create an internal pressure within its layers. Due to that phenomenon, the gap between graphene layers is being broadened allowing superior lithium diffusion, unveiling more active sites and increasing electric capacity.

The aim of this work was to create expanded reduced graphene oxide and tungsten disulfide (ERGO/WS₂) films at different ratios (1:1, 1:2 and 2:1), that would act as anode materials for lithium-ion half cells. The most efficient composite (ERGO/WS₂ (1:1)) showed improved cyclic stability, reversible capacity at lower current density and three times higher specific capacity, in contrast to thermally reduced RGO/WS₂ (1:1).

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Metal Organic Polymers as high-capacity energy storage material

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The unavoidable transition from fossil fuels to renewable energy sources together with the ever-growing worldwide energy demand have triggered the search for novel and efficient energy storage systems (ESS) that can support the transition and the energy supply for on-demand utilization. To this end, electrochemical energy storage technologies, and in particular rechargeable batteries and supercapacitors (SCs) hold great potential for technological breakthroughs in the field of energy.¹ Since their first commercialization by Sony in 1991, lithium-ion batteries (LIBs) have dominated the portable-electronics market. However, the limited and uneven distribution of lithium reserves across the globe has been recently acknowledged by EU Monitor, which identified lithium for the first time as critical raw material (CRM) in 2020,² sparking the development of new ESS relying on Na⁺, K⁺, Mg⁺, Al³⁺, Zn²⁺, etc.³

Metal-organic polymers (MOPs) have emerged as versatile organic materials for ESS due to their easily tunable structures, flexibility, low cost and well-dispersed single metal sites.⁴ The flexibility of polymeric materials makes it possible to insert/extract ions rapidly without significant volume change and therefore MOPs are capable of achieving fast ionic intercalations.⁵ In addition, their pore size, surface area and electrochemical activity can be easily tuned by the suitable choice of metal ions and organic ligands.

Herein, we present the synthesis of novel MOPs, Zn-TABQ and Cu-TABQ *via* the coordination of a redox-active monomer. Two different metal ions were used to explore and correlate their chemical structure with their electrochemical performance. A rechargeable Al ion battery was assembled, in which Zn-TABQ or Cu-TABQ were used as cathode materials, Al as anode and AlCl₃-[EMIm]Cl IL as electrolyte. Owing to the highly reversible conversion between the carbonyl and hydroxyl groups of TABQ, the Zn-TABQ and Cu-TABQ cathodes exhibit a remarkable electrochemical performance compared to other cathode materials in RABs.

This work was supported by the National Science Center Grant. No 2020/36/C/ST5/00247.

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Tuesday
September 13th, 2022

The detailed programme

Chair: Agnieszka Jastrzębska

9:15 - 9:50	Magdalena Birowska <i>Magnetic fingerprints in electronic and optical studies of 2D magnetic crystals</i>
9:50 - 10:25	Adam Babiński <i>Two-dimensional Semiconductors in Magnetic Field –Experimental Opportunities in the European Magnetic Field Laboratory</i>
10:25 - 10:40	Teresa Kulka <i>Magnetic properties of Ti₂C MXenes doped with transition metals Cr, Mn, and Fe</i>
10:40 - 10:55	Karol Szałowski <i>Electric field-controlled spin state in usthrene-like nanographenes: computational study</i>
10:55 - 11:25	Coffee
	Chairman: Maciej Molas
11:25 - 12:00	Artur Ciesielski <i>Two-dimensional materials as platform for water purification and sensing</i>
12:00 - 12:15	Daria Baranowska <i>Nanowired g-C₃N₄ for H₂ photogeneration from water splitting</i>
12:15 - 12:30	Anna Lewandowska-Andrałojć <i>Functionalization of Ti₃C₂T_x with dyes: spectroscopic insights and photocatalytic applications</i>
12:30 - 12:45	Bartosz Środa <i>ZIF-67/MXene composites as a highly efficient electrocatalyst for oxygen evolution reaction</i>
12:45 - 13:00	Dominika Bury <i>On the photocatalytic activity of the oxidation stabilized Ti₃C₂T_x MXene</i>
13:00 - 14:30	Lunch
	Chairman: Andrzej Wyszomółek
14:30 - 15:05	Barbara Piętka <i>2D-perovskites in microcavities: strong light-matter coupling regime and polariton condensate</i>
15:05 - 15:20	Agata Daniszewska <i>Technology of graphene flakes production via liquid phase exfoliation and their properties characterization</i>
15:20 - 15:35	Milena Ojrzyńska <i>Production of graphene flakes based on combined SO₃ intercalation-exfoliation method</i>
15:35 - 15:50	Jakub Rogoża <i>Metallic contacts and processing of epitaxial boron nitride</i>
15:50 - 16:05	Company presentation: Comef
16:05 - 16:35	Coffee
	Pause
18:45 - 19:45	Guided tour of the revitalized EC1 Power Plant
20:00 – 22:00	Dinner EC1 Łódź

Magnetic fingerprints in electronic and optical studies of 2D magnetic crystals

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In recent years, 2D magnetic materials gained a lot of interest due to their potential optoelectronics applications [1]. The current research focuses on the study of *the transition metal phosphorous tri-chalcogenides semiconductors* (MPX₃, M=1st row transition metals, X=chalcogenides), which are antiferromagnetic compounds exhibiting various magnetic orderings. These materials are stable in air, and we predict that the excitonic binding energies are giant for these compounds [2]. In fact, that these materials are 2D magnets, allowing one to both study and use magnetism and optics, and their interplay, in a single stable material. There is no precedence of such a platform in the realm of conventional materials.

In this study, we tackled a following scientific questions: what mechanism sustains the long-range AFM ordering, and whether the type of magnetic arrangement can be manipulated? Here, we report a comprehensive theoretical *ab initio* result of the electronic and optical properties of the series of MPX₃ monolayers (M=Mn, Ni, Fe, Co, and X=S,Se), as well as the alloy systems with magnetic [3] and nonmagnetic substitution [4]. In particular, for the AFM-Neel magnetic ordering, the inclusion of the spin-orbit interaction (SOI) causes an in-equivalency of the pair of valleys (K+,K-), resulting in sizeable valley splitting, which can be manipulated via the rotation angle of the spins. In the case of MnPS₃, MnPSe₃ and FePS₃ monolayers, we have demonstrated that the band edge direct transitions are optically active. In addition, we have reported an effective tuning of magnetic interactions and anisotropies in both MnPS₃ and NiPS₃ upon nonmagnetic substitution [4]. Such efficient engineering of the magnetism provides a suitable platform to understand the magnetism in thin samples.

We acknowledge support by the University of Warsaw "*Excellence Initiative - Research University*". Access to computing facilities of PL-Grid Polish Infrastructure for Supporting Computational Science in the European Research Space and of the Interdisciplinary Center of Modelling (ICM), University of Warsaw is gratefully acknowledged.

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Two-dimensional Semiconductors in Magnetic Field –Experimental Opportunities in the European Magnetic Field Laboratory

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Strong magnetic fields, both static and pulsed, provide numerous opportunities for studying, modifying and controlling the state of matter that researchers have at their disposal. This is of special importance in the case of emerging layered materials as e.g., transition metal dichalcogenides (TMDs) or perovskites. The effect of dielectric environment on the properties of excitons in TMD monolayers, the “brightening” of dark excitons in magnetic fields, which will be reviewed in this presentation, are examples of effects apparent in high magnetic fields.

The high field environments with well-equipped experimental setups and professional support by local researchers are available in the facilities of the European Magnetic Field Laboratory (EMFL). The structure was created as an answer to the fragmentation of infrastructure, duplication of research and innovation efforts in many centers and lack of coordination at the regional, national and international levels. The EMFL comprises three host members: High Magnetic Field Laboratories in France, (Grenoble, Toulouse), in Germany (Dresden), and in the Netherlands (Nijmegen). Experimental opportunities at EMFL as well as the modes of access to the infrastructures will be introduced.

The access of Polish users to the EMFL infrastructure is facilitated by the grant from the Ministry of Education and Science (DIR/WK/2018/2020/07-2) which also allows for the Polish membership in the EMFL. The grant is managed by the University of Warsaw on behalf of the Polish Consortium of Strong Magnetic Field Users. The Consortium, which is constantly open to new members, currently comprises: University of Warsaw, Institute of Physics, Polish Academy of Sciences (PAS); Institute of High Pressure Physics PAS; Łukasiewicz–the Institute of Microelectronics and Photonics, Institute of Molecular Physics PAS; Nencki Institute of Experimental Biology, PAS; Wrocław University of Technology, Włodzimierz Trzebiatowski Institute of Low Temperature sand Structure Research PAS, in Wrocław. Their activities and the concept of Regional Magnetic Field Laboratories will be presented.

Magnetic properties of Ti₂C MXenes doped with transition metals Cr, Mn, and Fe

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Two-dimensional titanium carbides Ti₂C, MXenes, have been attracted scientific effort, mostly owing to their promising applications. The magnetic moments of the external metallic Ti layers are ferromagnetically or antiferromagnetically oriented to each other depending on the remnants from the technological processes that cover the surface. The possibility to tune magnetic moments of the external MXenes layers through suitable functionalization could be utilized in numerous spintronic applications.

We have investigated the change of the magnetic properties of MXenes caused by the substitutional doping of Ti layers with transition metal (TM) atoms such as Mn, Cr and Fe. The introduction of TM atoms with different number of d-electrons (and therefore different magnetic moment) leads to breaking of the homogeneity of the spontaneous magnetization and formation of the skyrmionic-like patterns.

Our studies are based on the first principles calculations within the Kohn-Sham realization of the density functional theory (DFT) employing the Quantum Espresso computer package. We take spin-orbit interaction into account and therefore our calculations have to be performed in the non-collinear magnetism regime. To facilitate eventual future comparison with experiments, we have undertaken an attempt to compute the spin tunnelling current between the non-uniformly spin-polarized electrons of the MXenes surface and magnetic tip of the scanning tunnelling microscope (STM), in close analogy to codes providing the STM images from the electronic density obtained in DFT calculations.

Electric field-controlled spin state in uthrene-like nanographenes: computational study

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The on-surface synthesis of zigzag-edged nanographenes with atomic precision [1] invigorated the interest in theoretical modelling of such nanostructures, including also their magnetic properties. Significant attention is focused on diradical hydrocarbons, as the radical spins can take either singlet or triplet ground state. Recently, a successful synthesis of [7]uthrene [2], U-shaped nanographene molecule, and experimental confirmation of its magnetic triplet ground state attracted the interest to a class of uthrene-like nanographenes [3]. A highly interesting goal in the context of physics and applications of graphene nanostructures is the electric field control of their magnetism.

Our paper reports a computational prediction of the ground-state magnetic phase diagram of uthrene-based nanographenes in external in-plane electric field [4]. The model is based on Hubbard Hamiltonian in mean-field approximation, applied to charge-undoped molecules of uthrene, [7]uthrene and [8]uthrene. For all the considered structures, the states with total spin $S = 1$ are predicted in the absence of the electric field. The full phase diagrams include also electric field-induced $S = 0$ antiferromagnetic and non-magnetic states. The possibility of switching between these states with the electric field is predicted and the pronounced in-plane anisotropy of the necessary critical field is emphasized. The importance of uniaxial strain in the structures is discussed and the effect of the exchange field originating from the substrate on the phase diagram is evaluated.

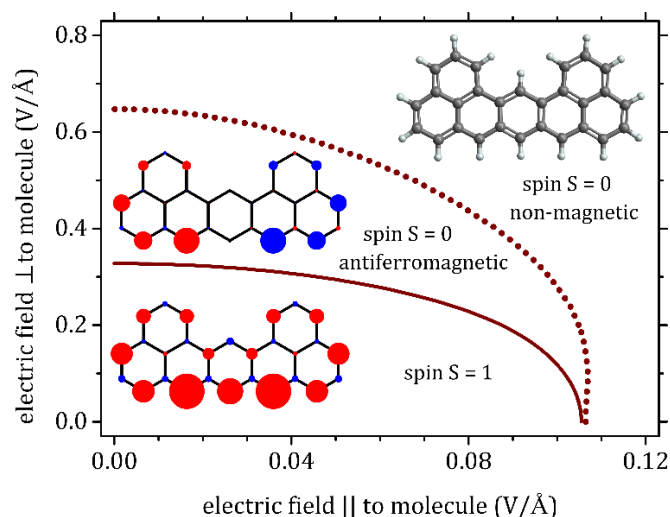


Fig. 1. Ground-state magnetic phase diagram for [7]uthrene in in-plane electric field.

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Two-dimensional materials as platform for water purification and sensing

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Two-dimensional materials (2DMs) exhibiting a high surface-to-volume ratio are unique scaffolds whose interactions with the environment drive their application as sensitive elements in chemical sensing. They allow prompt reconfiguration of the architectures of the sensor, whose response to the detection of chosen analyte becomes no longer limited by extrinsic factors such as the slow diffusion of target molecules through the active material or the presence of structural traps for small molecules/ions. The unique features of 2DMs determine the highest responsiveness, sensitivity, and reversibility combined with the lowest limit of detection in the sensing process.

Pristine 2DMs are being widely exploited as highly sensitive elements in chemical and physical sensors, although they suffer from the lack of intrinsic selectivity towards specific analytes. Here, we showcase the most recent strategies explored in our laboratories on the use of (supra)molecular interactions to harness selectivity of suitably functionalized 2D materials for chemical and physical sensing. We discuss how to achieve selectivity in chemical sensors along with other relevant characteristics, such as high sensitivity, response speed, and reversibility, by suitable functionalization and incorporation of low-dimensional materials into powerful transducers.

We will discuss piezoresistive pressure sensor based on a millefeuille-like architecture of reduced graphene oxide (rGO) intercalated by covalently tethered molecular pillars holding on-demand mechanical properties are fabricated. By applying a tiny pressure to the multilayer structure, the electron tunnelling ruling the charge transport between successive rGO sheets yields a colossal decrease in the material's electrical resistance. We will also discuss novel generation of humidity sensors based on a simple chemical modification of rGO with hydrophilic moieties, i.e., triethylene glycol chains. Such a hybrid material exhibits an outstandingly improved sensing performance compared to pristine rGO such as high sensitivity (31% increase in electrical resistance when humidity is shifted from 2 to 97%), an ultrafast response (25 ms) and recovery in the subsecond timescale, low hysteresis (1.1%), excellent repeatability and stability, as well as high selectivity toward moisture.

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Nanowired g-C₃N₄ for H₂ photogeneration from water splitting

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Due to interesting optical properties the photocatalysts such as TiO₂ ((rutile E_g = 3.0 eV), (anatase E_g = 3.2 eV)), MoS₂ (E_g = 2.4 eV), ZnO (E_g = 3.2 eV), CdS (E_g = 2.4 eV), and g-C₃N₄ (E_g = 2.7 eV) are commonly used in photocatalytic hydrogen generation. Among them, graphitic carbon nitride (g-C₃N₄) has attracted much attention due to its conjugated structure, suitable band gap tuning, good response to visible light, availability, and low price. Nevertheless, the g-C₃N₄ has an original bulk two-dimensional (2D) structure with low specific surface area and low light-induced carrier transfer efficiency, resulting in the suppression of photocatalytic applications [1]. To address the aforementioned issues and effectively increase the photocatalytic performance of starting g-C₃N₄, different preparation methods, including thermal condensation, solvothermal synthesis, microwave-assisted synthesis, ionic liquids, and molten salt strategies have been widely reported [2-5]. Additionally, considering the polymeric character of g-C₃N₄, and its ability to structural change, g-C₃N₄ with one (1D) and three dimensions (3D) are also studied. Generally, 1D g-C₃N₄ has a large specific surface area, strong light absorption capacity, excellent electron and hole separation ability, high aspect ratio, and fast carrier transport. In the case of 3D g-C₃N₄, the properties are the following: slow photon effect and rich pore structure [1]. Based on the above-mentioned 1D, 2D, and 3D g-C₃N₄ properties, 1D materials are the most desirable for photocatalytic applications.

In this contribution, a facile and eco-friendly preparation route of 1D g-C₃N₄ is reported. Initially, 2D g-C₃N₄ was modified in hydrothermal reaction leading to the formation of a 1D structure. The optimization of the preparation conditions toward boosting the photocatalytic H₂ evolution from water splitting reaction under simulated solar light illumination was conducted. For a deep understanding of the mechanism of photocatalytic reaction the morphology, chemical structure, optical and electrochemical properties were carefully investigated by several microscopic and spectroscopic techniques. The enhanced photocatalytic H₂ generation over the 1D g-C₃N₄ is achieved due to optimized optical band gap, enhanced light harvesting, the better position of valence and conduction bands toward photocatalytic hydrogen evolution, higher porosity, faster transfer and charge separation of photogenerated carriers, lower recombination rate resulting from 1D nanostructure.

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Functionalization of $Ti_3C_2T_x$ with dyes: spectroscopic insights and photocatalytic applications

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Photocatalysis is an appealing strategy to exploit solar energy for fuel production and pollutant utilization. Innovative 2D materials such MXenes with unique layered structures are expected to enhance photocatalytic activity due to excellent mobility of charge carriers and extremely high specific surface area [1]. In the last few years there has been increasing attention given to the interesting properties and fabrication of MXene or MXene-based photocatalysts for water splitting [1]. In our work by functionalizing for the first time non-covalently eosin Y and cationic porphyrin to $Ti_3C_2T_x$ we constructed novel nanomaterials that were characterized by spectroscopic methods (steady-state and time-resolved absorption and emission measurements). Our results clearly demonstrated that cationic porphyrin strongly interacts with MXenes in the ground state and excited state. Ti_3C_2 , though one of the most extensively studied 2D MXenes, was very rarely reported in dye-sensitized photocatalysis [2]. We also carried out photocatalytic hydrogen evolution experiment of the EY/ $Ti_3C_2T_x$ /CoSO₄ system under incident light wavelength. Hydrogen evolution rate of 40.9 mmol h⁻¹ g⁻¹ and AQE = 35.7% at 505 nm has been obtained which is even higher than for the analogue system in which CoSO₄ was replaced by the H₂PtCl₄ and higher than for the system where graphene oxide was used as a support.

Our work shows huge potential of 2D MXenes used in dye-sensitized photocatalysis for hydrogen evolution.

Acknowledgments: This work was supported by AMU "Excellence Initiative - Research University" (grant number: 038/04/NŚ/0038).

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ZIF-67/MXene composites as a highly efficient electrocatalyst for oxygen evolution reaction

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Nowadays fossil fuels are exhaustible, climate changes are progressing due to pollution people-made, this is why we need to find an alternative source of clean energy. What so more they are very important aspects for the scientist [1]. For many years researchers are looking for a new low-cost and environmentally friendly way to produce energy. One of the simplest, most efficient sources of power is fuel cells, water splitting and CO₂ conversion [2]. Oxygen evolution reaction (OER) by electrocatalytic water splitting is necessary for efficient electrochemical energy storage.

The aim of this contribution was the preparation of composites made from ZIF-67 (Zeolitic Imidazolate Framework-67) and MXene. First, both structures were dispersed in methanol, and then two solutions were mixed under sonication. Finally, the produced samples were dried under the vacuum dryer. The detailed characterization of the composites was performed via scanning electron microscopy, X-ray diffraction, Raman and FTIR spectroscopy. Moreover, the samples were tested as electrocatalysts for OER. We obtained low overpotential 69,2 mV at 1 mA/cm² and 366,6 mV at 10 mA/cm². Figure 1 was presented the image of ZIF/MXene composite (weight ratio: 1 MXene : 10 ZIF-67).

Acknowledgements: This work was financially supported by National Science Centre Poland (Preludium Bis 2, 2020/39/O/ST5/01340).

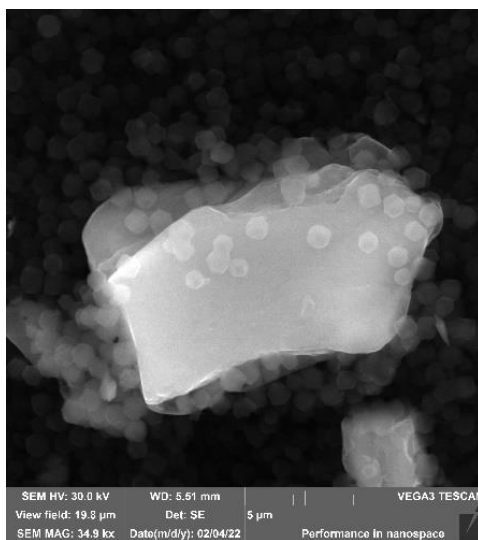


Fig 1. SEM image of ZIF/MXene 1_10 composite.

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On the photocatalytic activity of the oxidation stabilized $Ti_3C_2T_x$ MXene

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Two-dimensional (2D) nanomaterials are characterized by unique optical properties such as superior light absorption and direct to the indirect band gap. For this reason, scientists have found many potential applications for them in the photocatalysis process, which can be utilized in organic dye decomposition, environmental engineering, and protecting the environment [1]. One of the most interesting groups of 2D nanomaterials are transition metal carbides or nitrides called MXenes with the formula of $M_{n+1}AX_n$, where M is a transition metal, A is an A group element, X is a carbon or/and nitrogen, while $n = 1-3$ or even 4 [2].

However, MXenes are relatively unstable and difficult to control during the photocatalysis process [3]. In our work, we synthesized $Ti_3C_2T_x$ MXene *via* two well-established approaches such as HF/TMAOH and minimum intensive layer delamination with HCl/LiF. Further, we stabilized obtained nanostructures with L-ascorbic acid (Vit.C) to prevent oxidation. Next, we analyzed the optical properties of $Ti_3C_2T_x$ MXene and obtained excellent results. We utilized them to the photocatalytic decomposition of methylene blue, bromocresol green, and the commercial blend of textile dyes, using simulated daylight and UV light. Our results shown almost 100% effectiveness in the purification of dyes with four swift actions. Furthermore, analysis at various visible light ranges showed that irradiation with 625 nm (red light) gave the highest efficiency of the process. We also checked the mechanism of decomposition dyes, especially action concerning surface functional groups, dye adsorption on the $Ti_3C_2T_x$ MXenes' surface, and the activity of reactive oxygen species (ROS). Furthermore, we noticed that the photocatalysis process did not influenced the structure and morphology of MXenes. Finally, the photocatalysts were regenerated and successfully reused.

Acknowledgments: The presented results were accomplished thanks to the funds allotted by the National Science Centre, within the framework of the research project 'OPUS 16' no. UMO-2018/31/B/ST3/03758 and POB Technologie Materiałowe of Warsaw University of Technology within the Excellence Initiative: Research University (IDUB) program.

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2D-perovskites in microcavities: strong light-matter coupling regime and polariton condensate

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Exciton-polaritons in organic and inorganic perovskites open a new path towards polaritonic devices working at room temperature with strong nonlinear effects. In particular, the 2D-perovskites that crystalline structure is equivalent to multitude of QW with controlled width, makes them particularly interesting for strong light-matter coupling. I'll demonstrate the formation of polariton modes in an optical cavity filled with 2D-perovskites and discuss the implications of this effect for polariton condensation. Moreover, I'll present a novel architecture of a microcavity with perovskites and a highly birefringent liquid crystal (LC) (Fig. 1 a), where the birefringence is controlled by external electric field and the strong light-matter coupling condition is achieved with subsequent cavity modes. We drive the system through polaritonic H-V split modes (Fig. 1 b, c) and spin-orbit coupled modes of Rashba-Dresselhaus (R-D) type (Fig. 1 d, e). Another important property of our structure is the non-trivial band geometry that appears due to additional birefringent anisotropy coming from the LC. It allows us to lift the degeneracy at the Rashba-Dresselhaus crossing point (Fig. 1 f) and open the gap at two diabolical points with the Dirac cone-like dispersion relation (Fig. 1 g, h) demonstrating the emergence of non-zero local Berry curvature. The polariton condensate at room temperature is revealed in all regimes allowing to directly implement this structure in devices requiring non-linear signal processing at room temperature.

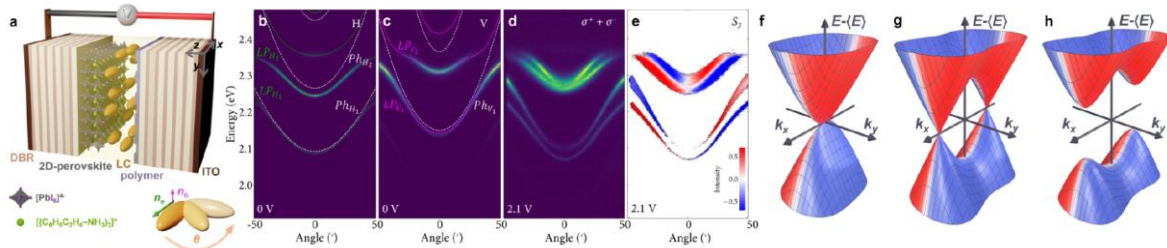


Fig. 1. a) Scheme of a microcavity containing a 2D-perovskite and liquid crystal. b, c) Polariton emission spectra in for H-V split modes and d) in R-D SOC regime with e) S3 Stokes component. f) Energy of the modes subtracted by their mean value $\langle E \rangle$ in R-D regime, g) for positive detuning of the photonic modes from R-D resonance and h) for broken inversion symmetry due to additional birefringence.

Technology of graphene flakes production via liquid phase exfoliation and their properties characterization

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Liquid phase exfoliation of different graphite materials was carried out in microfluidization process using high pressure homogenizer. The influence of exfoliation process on the material's physico-chemical properties was verified. Size and thickness of produced graphene flakes are characterized using Raman spectroscopy, DLS, XRD, SEM, AFM and TGA analysis. Comparison of exfoliation progress for different input graphite materials is performed based on the correlation between all presented characterization methods.

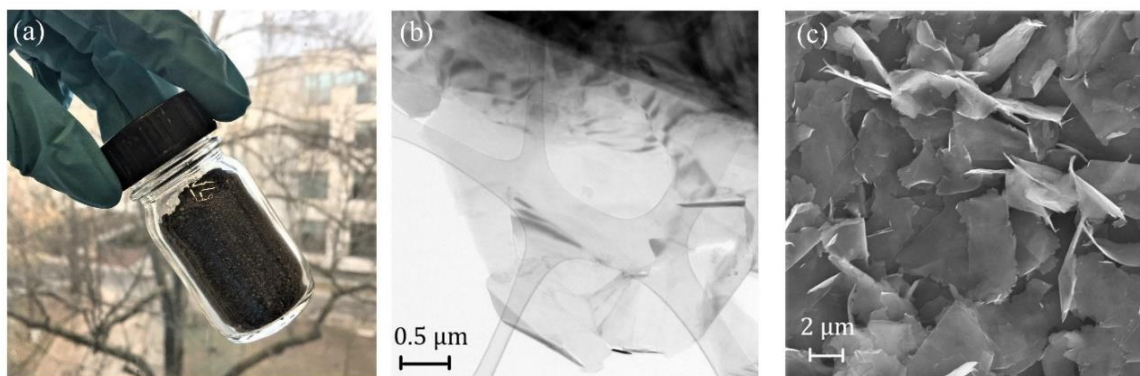
Production of graphene flakes based on combined SO₃ intercalation-exfoliation method

M. Ojrzyńska¹, A. Daniewski¹, A. Dużyńska¹, M. Zdrojek¹

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High quality and high yield production of graphene flakes is the goal of today's graphene technology that would allow commercialization and industrialization. Recently developed innovative methods still suffering from low quantities, controllable qualities, processability, and costs [1]. Here, we developed a simple, yet compelling chemical route for industry-scale production of few-layer graphene that rely on simultaneous non-oxidative intercalation and exfoliation of raw graphite in oleum with nearly 100% efficiency, one of the highest ever reported. High yield is enabled because un-bounded SO₃ molecules dissolved in sulfuric acid can effectively intercalate the graphite boosting spontaneous exfoliation and providing undefected, thin graphene flakes. The X-ray and vibrational spectroscopy confirm the absence of defects and oxides in the graphene layers and the electron microscopy and diffraction method show the structure.

Acknowledgments: This research was supported by the PRELUDIUM BIS project (UMO 2019/35/O/ST5/01440).



[1] Lin, Li & Peng, Hailin & Liu, Zhongfan. *Nature Materials*. **18**. 520-524 (2019).

Metallic contacts and processing of epitaxial boron nitride

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Hexagonal boron nitride (h-BN) is a very promising candidate for optoelectronic applications in the deep ultraviolet spectral range due to its exceptional physical properties, such as high chemical stability [1], thermal conductivity [2] and wide bandgap energy [3]. A large cross section for neutron capture renders BN an outstanding candidate for neutron detectors [4]. However, obtaining micro-scale devices on epitaxial h-BN layers is a challenge due to wet delamination that may occur during typical process steps.

In this communication we present a new method of preparation of h-BN layers for optical lithography. Our technique prevents delamination of material from sapphire substrate during the etching as well as metal coating processes. Additionally, it generates much less wrinkles on the processed h-BN. Fig. 1 shows a h-BN hall-bar etched with reactive ion etching. In the next stage metallic contacts made out of AuPd alloy were sputtered on the structure. Before the actual processing, the sample was prepared according to our method, which is based on the removal of wrinkles by controlled delamination. The image illustrates that our method allows us to perform multi-stage (multiple etching and sputtering) processes on thin layers of epitaxial h-BN. Electrical and optoelectrical measurements of the obtained structures will be discussed.

This work was partially supported by the National Science Center of Poland, grants no 2019/33/B/ST5/02766, 2021/41/N/ST7/04326.

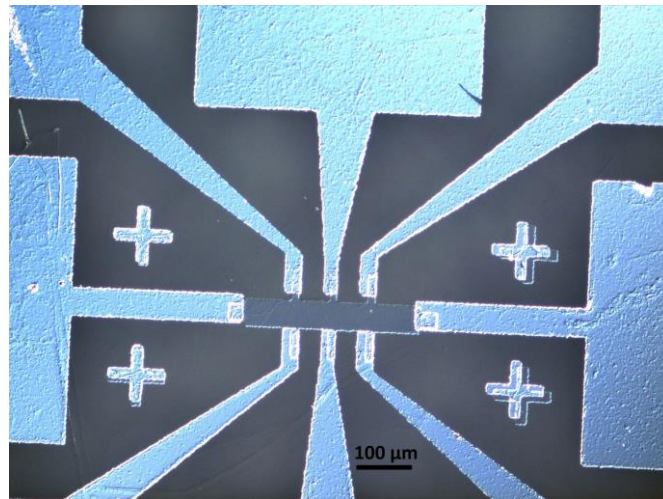


Fig 1. Optical image of h-BN hall bare structure with AuPd electrodes. The structure was created in a 2 stage lithographic process.

- [1] N. Kostoglou, et al. *Vacuum* **112**, 42 (2015).
- [2] J. Zheng, et al. *2D Materials* **3**, 11004, (2016).
- [3] G. Cassabois, et al. *Nature Photonics* **10**, 262–266 (2016).
- [4] A. Maity, et al. *Applied Physics Letters* **114**, 222102 (2019).

Wednesday
September 14th, 2022

The detailed programme

Chairman: Adam Babiński

9:15 - 9:50	Agnieszka Jastrzębska <i>Novel and intriguing two-dimensional MBenes</i>
9:50 - 10:25	Madhurya Chandel <i>A novel and reproducible approach for the synthesis of MBene</i>
10:25 - 10:40	Michał Jakubczak <i>Nb-MXenes bioremediation with green microalgae: The mechanism of action and a road to decomposition</i>
10:40 - 10:55	Muhammad Purbayanto <i>Tunable Antibacterial Activity of a Polypropylene Fabric Coated with Bristling Ti3C2Tx MXene Flakes Coupling the Nanoblade Effect with ROS Generation</i>
10:55 - 11:25	<i>Coffee</i>
	Chairman: Martin Gmitra
11:25 - 12:00	Agnieszka Stępniań-Dybala <i>Silicene formations on Pb-Si heterostructures</i>
12:00 - 12:15	Jozef Haniš <i>Quasiparticle Interference in Superconducting Layered Misfit Compounds (LaSe)_{1.14}(NbSe₂)_x, x=1,2.</i>
12:15 - 12:30	Jakub Kierdaszuk <i>Gating and electrostatically-induced strain of graphene on nanorods</i>
12:30 - 12:45	Małgorzata Giza <i>Influence of 2-dimensional interlayers on contact resistance in TMDs-based field-effect transistors</i>
12:45 - 13:00	Maxime Le Ster <i>Moiré superlattices in reciprocal space</i>
13:00 - 13:10	Conference closing
13:10 - 14:30	<i>Lunch</i>

Novel and intriguing two-dimensional MBenes

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Two-dimensional MBenes currently emerge as promising post-MXene materials. They are a derivative of ternary MAB-phases and represent a new member in the flatland. However, MBenes differ in many ways from MXenes. Compared to MXenes, MBenes' structure appears to be more complex due to multiple crystallographic arrangements, polymorphism, and structural transformations. Consequently, this makes their synthesis and subsequent delamination into single flakes challenging.

Nevertheless, MBenes hold great potential for various applications due to having boron in their structure, rich structural chemistry, excellent reactivity, mechanical strength/stability, electrical conductivity, transition properties, and energy harvesting possibilities, just to mention a few. Therefore, exploring their activity and response in various fields seems plausible, as supported by theoretical calculations and preliminary experimental attempts.

Moreover, MBenes bear tremendous biotechnological potential. It is expected that the presence of boron in MBenes' structure could significantly change the interactions with biological matter, which needs careful attention and verification. Their interesting bioactive and functional features such as light-to-heat transition properties, which are highly relevant for PTT procedures with near-infrared (NIR) transition, photoacoustic and magnetic resonance imaging (MRI) of tumor sites as well as multimodal imaging-guided photothermal therapy, are expected to boost more fundamental research towards the exploration of MBenes' bioactive features in the next decade.

Collectively, the increasing number of practical applications will rapidly develop for 2D MBenes. In upcoming years, MBenes will pursue their counterparts - 2D MXenes. Further innovations in MBenes' post-processing approaches will allow the designing of new functional systems and devices with multi-purpose functionalities, thus opening a promising paradigm for the conscious design of high-performance 2D materials.

Acknowledgments: The presented results were accomplished thanks to the funds allotted by the National Science Centre, within the framework of the research project 'OPUS 18' no. UMO-2019/35/B/ST5/02538.

A novel and reproducible approach for the synthesis of MBene

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MBenes are early transition metal borides and a new two-dimensional (2D) material class. In 2015, Ade and Hillebrecht introduced their first rational classification. Considering MBenes' name and structure, it is believed that they are MXene-type materials. However, they differ in many ways. MBene's structure seems more complex due to multiple crystallographic arrangements, while the presence of boron and transition metal-boron chemistry changes its reaction pathway and structural transformations. [1]

Since the high oxidation susceptibility of MBenes, the conventionally tested wet chemical etching methods become challenging. In particular, they require a long and difficult-to-control procedure and thus are limited to producing only oxy-borides from their corresponding MAB phases. Therefore, we decided to apply the microwave-assisted hydrothermal method to synthesize MBenes. This hands-on method is precise and allows to control of the final product's size and shape distribution, crystallinity, and avoiding oxidation by adjusting the process parameters. The microwave-assisted hydrothermal method also yields a uniform and homogeneous product, which is another critical asset. [2]

As per literature and theoretical results, MBenes are another important 2D materials. They have lots of capabilities that can be useful for different applications because of having boron in their 2D structure. [1-2] If synthesized in a reproducible manner and in larger amounts, MBenes may take the place of MXene/graphene in the future. Our findings and exploration of MBenes may generate new paths for easier handling of high-performance 2D materials.

Acknowledgments: The presented results were accomplished thanks to the funds allotted by the National Science Centre, within the framework of the research project 'OPUS 18' no. UMO-2019/35/B/ST5/02538.

[1] M. Jakubczak, A. Szuplewska, A. Rozmysłowska-Wojciechowska, et al. *Advanced Functional Materials*, **38**, 2103048 (2021).

[2] Z. Jiang, P. Wang, X. Jiang, et al. *Nanoscale Horizons* **3**, 335-341 (2018).

Nb-MXenes bioremediation with green microalgae: The mechanism of action and a road to decomposition

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The two-dimensional (2D) early transition metal carbides, nitrides, and/or carbonitrides called MXenes attract scientific attention due to their intriguing morphology and unique properties. MXenes are obtained by top-down selective etching of A element from parental $M_{n+1}AX_n$ phases, in which M represents an early transition metal, A stands for an element from group 13 or 14 of the periodic table, X is carbon and/or nitrogen, while $n=1, 2, 3$ or 4. Further delamination of as-synthesized MXene with accordion-like morphology allows obtaining few or single layer nanoflakes, which reminds graphene [1]. Their low bio-transformation susceptibility and the lack of understanding of material surface-organism interactions do not allow however to take full advantage of MXene's application potential.

In our work, we developed a facile approach to track potential roads of bio-remediation of Nb-based MXenes with green microalgae. For this purpose, we utilized 2D Nb_2CT_x and $Nb_4C_3T_x$ MXenes as model inorganic crystalline contaminants. Further, we checked how their presence in the water environment affects the growth of green microalgae *Raphidocelis subcapitata*. As we have found, a slight initial reduction of microalgae growth went side-by-side with their recovery ability within 72 hours of water treatment. Further tests confirmed that microalgae could decompose Nb-MXenes due to surface-related physicochemical interactions. X-ray photoelectron spectroscopy proved that initially attached to the surface of microalgae Nb-MXenes were decomposed into NbO and Nb_2O_5 . Interestingly, microalgae readily consumed Nb-oxides, which seemed to be non-toxic for them. However, microalgae did not just walk past the observed nutritional effect. We noticed their increased size, smoothed shape, and higher growth rates with dynamic particle shape analysis and SEM observations. In general, utilized green microalgae proved themselves as a superior tracking system for even negligible ecosystems contamination with tested materials. Moreover, we laid the groundwork to answer the questions about the impact of Nb-MXenes on the water environment, their bio-remediation, and associated surface interaction between inorganic crystalline nanomaterials and water organisms.

Acknowledgments: The presented results were accomplished thanks to the funds allotted by the National Science Centre, within the framework of the research project 'SONATA BIS 7' no. UMO-2017/26/E/ST8/01073.

[1] M. Naguib, M. Kurtoglu, V. Presser, et al. *Advanced Materials* **23**, 4248-4253 (2011).

Tunable Antibacterial Activity of a Polypropylene Fabric Coated with Bristling $Ti_3C_2T_x$ MXene Flakes Coupling the Nanoblade Effect with ROS Generation

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Polypropylene (PP) is a thermoplastic polymer widely used as a medical textile in healthcare applications due to its low cost and superior performance. However, it does not show antibacterial properties leading to the possibility of pathogen transmission [1]. Herein, we have developed an antibacterial medical fabric by facile self-assembly of delaminated two-dimensional (2D) $Ti_3C_2T_x$ MXene flakes bristling on the surface of PP fibers. The increasing amount of MXene in the coating solution from 1 up to 32 mg/mL allowed for edge-on assembly of MXene flakes on the PP surface and tracking the evolution of the band gap for a restacked structure. Characterization of the PP/ $Ti_3C_2T_x$ nanocomposite has proven that it exhibited highly effective antibacterial, robust coating, and chemically/thermally stable properties. The *in vitro* microbiological studies against Gram-negative *Escherichia coli* and Gram-positive *Staphylococcus aureus* have shown that PP/ $Ti_3C_2T_x$ reduced the bacterial viability up to 100%, as driven by synergistic membrane stress mediated by physical contact and light-induced reactive oxygen species (ROS) generation [2]. Moreover, the use of L-ascorbic acid for MXene stabilization allowed for achieving excellent thermal stability of the PP/ $Ti_3C_2T_x$ nanocomposite upon accelerated thermal aging. Collectively, this work provides a facile surface engineering strategy for designing medical fabrics with outstanding functional performances. By demonstrating the exceptional performance of the stabilized MXene in a self-assembly nanocomposite structure, we are opening the door for MXenes to be applied in other biomedical fields.

Acknowledgments: The microbiological-related studies, material preparation, and characterization were accomplished thanks to the funds allotted by the National Science Center, within the framework of the research project “OPUS-18” (UMO-2019/35/B/ST5/02538). The light irradiation tests were performed within research funded by POB Technologie Materiałowe of Warsaw University of Technology within the Excellence Initiative: Research University (IDUB) program. M.J. and D.B. also acknowledge financial support from the IDUB project (Scholarship Plus program).

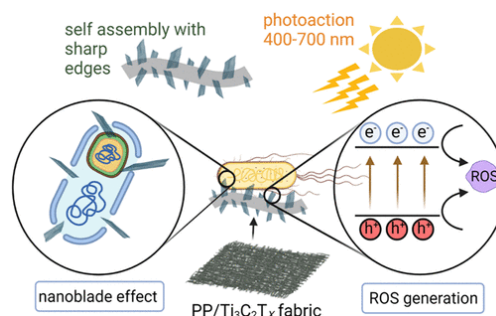


Fig. 1. The schematic diagram of antibacterial mechanism in PP/ $Ti_3C_2T_x$ nanocomposites.

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[2] Purbayanto, M. A. K., Jakubczak, M., Bury, D., et al. A. ACS Applied Nano Materials, **5**(4), 5373–5386 (2022).

Silicene formations on Pb-Si heterostructures

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Silicon is the basis of present semiconductor industry. The question arises: can any specific form of this traditional material, compatible with current semiconductor technology, be used in next-generation nanoelectronics? The answer here seems to be silicene, a two-dimensional material made of silicon atoms arranged in a honeycomb-type crystallographic lattice [1]. Like its predecessor, graphene, it is characterized by linear dispersion bands that form Dirac cones, giving its new properties. The main difference between the two materials is that silicene does not occur in a layered form. Silicene production is a process that requires the control of many factors such as sample temperature or the deposition rate of Si atoms. All these factors must be tuned and optimized according to the substrate used. Up to now it has been possible to synthesize silicene in epitaxial form, i.e., as a result of deposition of a layer of silicon atoms [2,3] and in the process of segregation of Si atoms on the surface of some metals [4]. However, the presence of a metallic substrate and interaction between them can significantly modify both the electronic structure of silicene and the material used. If we replace the substrate material with a superconductor, then owing to the phenomenon of proximity, it will be possible to create systems in which relativistic physics with Dirac quasiparticles and superconductivity with Cooper pairs are in contact. To date, however, there is a lack of systematic studies of the influence of silicene layers on superconductivity. It can be assumed that as a result of the proximity effect, superconductivity will 'penetrate' into silicene and this will become superconducting, but on the other hand, silicene can also act as a barrier to Cooper pairs and thus affect superconductivity in Pb. In view of these issues the knowledge of interfacial properties of silicene/Pb structures is of prime importance.

We study the formation of silicene layers on Pb-Si heterostructures and Pb(111) crystal. We use combined Low Temperature-Scanning Tunneling Microscopy/Spectroscopy (LT-STM/STS) and DFT calculations to characterize structural and electronic properties of the system at liquid helium temperatures. Our STM/STS investigations reveal that Si deposited onto $\sqrt{3}\times\sqrt{3}$ -Pb surface forms nanoribbons, directly bonded to the Si(111) substrate. While the deposition of silicon on the Pb substrate results in two different Si phases: $\sqrt{3}\times\sqrt{3}$ covered and 1×1 uncovered silicene structures. The results of preliminary research on Si on Pb(111) suggest that Si was covered with a Pb layer (at least one).

[1] K. Takeda, K. Shiraishi, *Physical Review B* **50**, 14916 (1994).

[2] P. Vogt, P. De Padova, C. Quaresima, et al. *Physical Review Letters* **108**, 1555501 (2012).

[3] B. Feng, Z. Ding, S. Meng, et al. *NanoLett.* **12**, 3507–3511 (2012).

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Quasiparticle Interference in Superconducting Layered Misfit Compounds $(\text{LaSe})_{1.14}(\text{NbSe}_2)_x$, $x=1,2$

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Unconventional superconductivity in transition metal dichalcogenides exhibits a special form of Ising pairing mechanism, with interesting consequence where the in-plane upper critical magnetic field is much higher than the Pauli limit. Misfit layered systems $(\text{LaSe})_{1.14}(\text{NbSe}_2)_x$, $x=1,2$ are a stack of transition metal dichalcogenide NbSe_2 layers intercalated by the LaSe layers. The system is a bulk superconductor indicating a unique three-dimensional Ising superconductor. We investigate possible quasiparticle interference patterns relevant for Fourier-transform scanning tunneling spectroscopy. We discuss the effect due to scalar and magnetic impurity in normal and superconducting states for conventional and unconventional pairing parameters using the T-matrix approach. For electronic structure we employ a tight-binding model fitted to the first-principles calculations.

This work was supported by the project APVV SK-PL-21-0055, VEGA Grant No. 1/0105/20, Slovak Academy of Sciences project IMPULZ IM-2021-42 and project FLAG ERA JTC 2021 2DSOTECH.

[1] X. Xi et Al., *Nature Physics* **12**, 139 (2016).

[2] P. Szabó et al., *Phys. Rev. Lett.* **86**, 5990 (2001).

[3] D. Sticlet, C. Morari, *Phys. Rev. B* **100** 075420 (2019).

[4] C. Bena, S. A. Kivelson, *Phys. Rev. B* **72** 125432 (2005).

Gating and electrostatically-induced strain of graphene on nanorods

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Graphene nanoresonators and gated structures have been proposed as efficient platforms for the fabrication of optomechanical devices, sensors, and mass sensing [1]. In the most widely used capacitor geometry, graphene is deposited on holes etched in a dielectric medium which separates graphene from a bottom conductive substrate. In this work, we demonstrated an alternative approach in which the four-layer graphene (4Lgr) is deposited on GaN nanowires. The 4Lgr electrode offers higher durability and lower resistivity as compared to a graphene monolayer. Moreover, our recent work underlined the high usefulness of GaN substrate (consisting of the 100 nm of undoped GaN grown on highly n-doped GaN) for effective graphene gating [2]. The etching of nanorods in the GaN substrate by plasma treatment changes the properties of the 4Lgr/GaN device. As demonstrated by the Raman spectroscopy, the bias applied between the graphene and nanorods affects the graphene electrode in two ways: a) by changing the electron concentration and b) by inducing strain (Fig. 1). The shift of graphene Raman modes observed under bias clearly shows the presence of electrostatically induced strain and only weak modification of carrier concentration. Due to the reduced contact surface, the efficiency of graphene gating is one order of magnitude lower than for a comparable structure without nanorods. Kelvin probe atomic force microscopy measurements show that morphology of graphene and distribution of carrier concentration are independent of gate bias. Therefore, we suspect that the screening effect in 4Lgr is responsible for the absence of both effects in the upper graphene layers. The higher impact of bias on strain was observed for samples with a larger area of contact between graphene and GaN nanorods which shows perspective for the design of graphene nanoresonators.

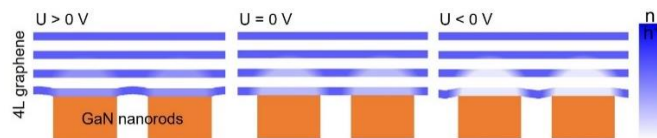


Fig. 1. Scheme of carrier concentration distribution and morphology of 4Lgr on GaN nanorods at different biases. Efficient interaction occurs only at the bottom graphene layer.

[1] Weber, P.; et al., *Nature Communications* **7**, 1, 12496, (2016).

[2] Kierdaszuk J., et al., *Applied Surface Science* **560**, 149939 (2021).

Influence of 2-dimensional interlayers on contact resistance in TMDs-based field-effect transistors

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The electrical contacts to two-dimensional semiconductors such as Transition Metal Dichalcogenides are still a main limiting factor in devices performance. This significant bottleneck in an efficient current injection into the 2D active layers is due to the formation of the Schottky barrier (SB). The formation of the Schottky barrier is governed by two main factors. One, the classical approach describes the simple difference between the electron affinity of the semiconductor and the work function of the metal. Two, when the interface is rich in carrier traps the SB height no longer follows the above-mentioned relation, and this effect is called Fermi level pinning (FLP). Due to this effect, the SB cannot be controlled by changing the contact material (changing the work function). Thus, to avoid this problem one can put an additional layer between the metal and 2D semiconductor in order to unpin the Fermi level and make it possible to control the SB height [1].

In this study, we explore the various configurations of the interlayer relying on different kinds of materials. For this purpose, using the gold-assisted mechanical exfoliation method [2] we produce large-area TMDs monolayers, which are shaped with e-beam lithography and dry etching. The large area of the material enables the fabrication of multiple devices on the same layers, allowing for a reliable comparison of their performance. Using a PDMS-based transfer system, the additional layer is placed only on the contact area of the device. Then the metal layer is thermally evaporated on top of the contact structure. In this way, we obtain a monolayer back-gate transistors with a 2D interlayer under metal contact (Fig.1 left). Our devices are designed in TLM architecture (Fig.1 right) with channel lengths under 1 μm , which allows us to accurately determine the contact resistance. The results of this work contribute to improvement in contact engineering strategy which leads to enhanced performance of 2D TMDs-based devices.

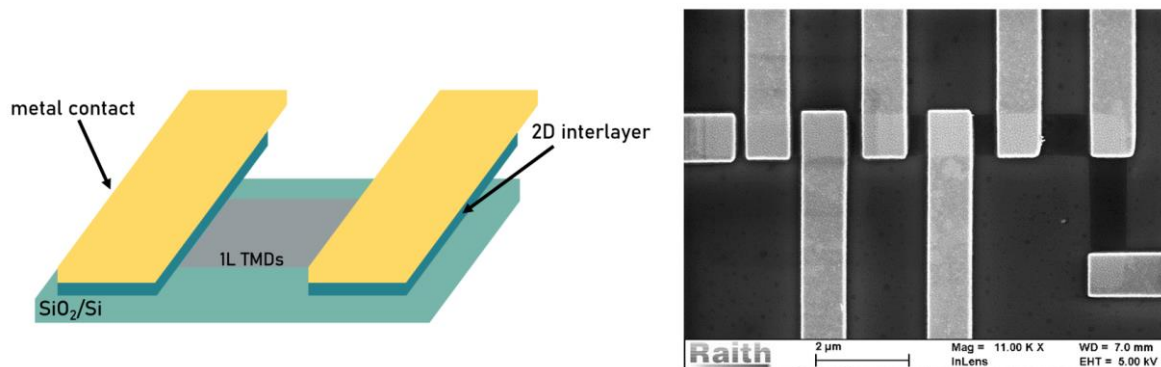


Fig. 1 (Left) Schematic of the transistor with 2D interlayer, (right) SEM image of TLM structure.

[1] K. Andrews, A. Bowman, *ACS Nano* **14**, 5 (2020).

[2] F. Liu, W. Wu, *Science* **367**, 6480 (2020).

Moiré superlattices in reciprocal space

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Moiré superlattices are ubiquitous in the study and investigation of two-dimensional (2D) materials. They emerge due to the broken (or modified) translational and rotational symmetries that exist in the otherwise uncoupled individual lattices. The consequences of the moiré superlattice on the optical and electronic properties is the subject of an increasing number of investigations [1, 2], and the most discussed emerging property is the presence of both unconventional superconductivity and Mott insulator states in twisted bilayer graphene [3, 4]. Many other moiré properties have been uncovered including ferromagnetism, moiré excitons, moiré solitons, moiré topological states, etc. The theory of these phenomena is under intense debate, and in this presentation, I will introduce a novel plane wave reconstruction method that explains the emergence of moiré coupling in 2D materials [5]. The new model allows to describe with a high degree of fidelity the moiré superlattices present in the scanning tunnelling microscopy images in a variety of van der Waals-bonded multilayer systems.

Acknowledgements: This work was supported by National Science Centre, Poland under the project No. 2019/35/B/ST5/03956 and UŁ 6/JRR/2021 grant.

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Poster Session
Monday September 12th, 2022

The detailed programme

P01	Chrobak Maciej <i>Tuning the Fermi level into a bulk energy gap by varying the Te amount in non-stoichiometric Bi_{2-x}Te_{3+x} crystals</i>
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P09	Nowak Ewelina <i>The influence of aminoalcohols on structure of ZnO thin films synthesized with sol-gel method</i>
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P11	Przybysz Przemysław <i>The DFT calculation of the interactions between graphene and Td-WTe₂</i>
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P13	Toczek Klaudia <i>Growth and oxidation of bismuthene on van der Waals substrates</i>
P14	Warda Krzysztof <i>The fast demagnetisation process in magnetic ultra-thin films by very short laser pulse of high power</i>
P15	Żuberek Ewa <i>Investigations of exciton-trion and exciton-biexciton coupling in van der Waals hBN/WS₂/hBN heterostructures by upconversion photoluminescence excitation measurements</i>

Tuning the Fermi level into a bulk energy gap by varying the Te amount in non-stoichiometric Bi_{2-x}Te_{3+x} crystals

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P01

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Bismuth telluride is one of the 3D topological insulators (TI) that can be characterized as materials having an insulating volume, while the surface remains conductive. At the interface between the TI and the trivial insulator (e.g., vacuum), the bulk energy gap is closed by surface metallic states with a linear dispersion relation (Dirac states). The practical use of these topological properties requires fine tuning of the Fermi level with respect to the energy gap in the bulk electronic states. Apart from doping with foreign elements [1], this tuning might be also achieved by making non-stoichiometric materials of the Bi_{2-x}Te_{3+x} type. Therefore, the aim of our work is to determine the influence of the Te amount on electronic transport, including analyses of the Shubnikov-de Haas (SdH) oscillations, the local electronic structure and the surface morphology.

Based on electronic transport measurements performed in sub-Kelvin temperatures (~100 mK) and in magnetic fields up to 14 T, we can say that all the tested samples reveal SdH oscillations, which proves a good quality of the investigated single crystals and a high mobility of the carriers. The Fast Fourier transform analysis of the stoichiometric sample shows that we can distinguish two frequencies, 12 T and 27 T, in the SdH oscillations, and thus there are two extremal Fermi surfaces with different Fermi wave vectors. The Berry phase of these frequencies obtained from the Landau Level Fan diagram is π and 0, respectively. It can be concluded that the lower frequency originates from the surface states with a linear dispersion relation and the higher frequency comes from the trivial bulk states. Then, along with increasing the Te concentration, we observed that the SdH oscillation frequencies were changing, thus the Fermi level was shifting. This effect was also confirmed by examining the Hall effect and examining the local electronic structure by the STS technique with a scanning tunnelling microscope. The most promising results were obtained for the sample with $x = 0.0173$. The SdH oscillations show that the frequency which comes from the surface states is dominant and the bulk frequency is almost invisible. This result indicates that the Fermi level is in the bulk energy gap or that it lies on the edge of the valence band.

Our results show that it is possible to tune the Fermi level so that it is in the bulk band gap by changing the crystal stoichiometry, and therefore it might be possible to use the properties of the non-trivial topology of the surface states of 3D topological insulators.

Acknowledgments: K.N. was partly supported by the EU Project POWR.03.02.00-00-I004/16.

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Supercapacitors based on graphene oxide enriched with thioamide based polymer

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P02

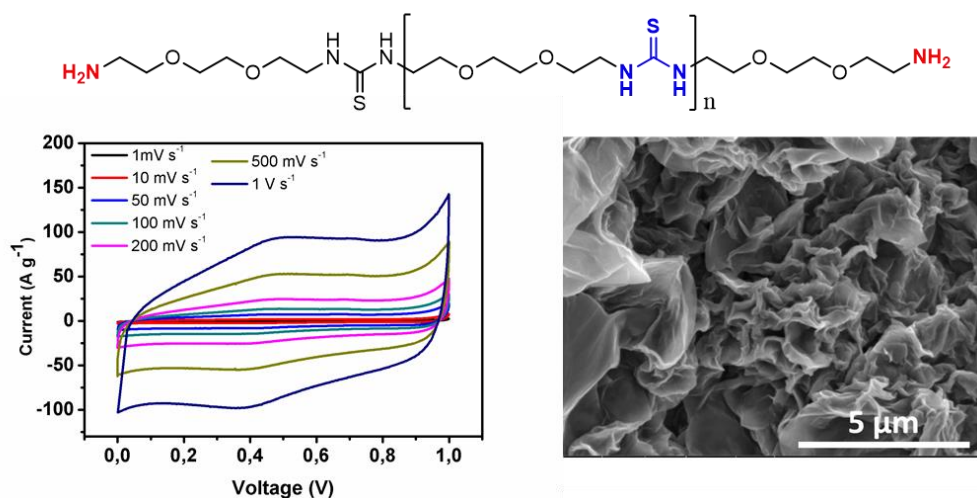
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Graphene oxide (GO) exhibits unique characteristics such as high mechanical strength or large surface area and provides low-cost, scalable alternative to graphene.[1] Furthermore the presence of oxygen-rich functionalities provides excellent water dispersibility and allows its covalent/non-covalent functionalization. Supercapacitors have recently gained significant attention as high-surface-area conducting materials possessing high power density, ultrafast charge-discharge rate, long cycle life, great stability and low maintenance.[2] Introduction of heteroatoms (e.g. N,O,S,P) into the graphene-based materials can significantly increase capacity performance of carbon materials by contributing additional pseudocapacitance through surface Faradic redox reactions.[3] Therefore we synthesized and characterized a novel 3D hybrid material of graphene oxide (GO) covalently functionalized with thioamide based polymer.

Modification of GO with the polymer leads to highly porous material with specific area reaching 320 m² g⁻¹ that exhibited significant results of the capacitance while tested in aqueous and organic electrolytes. The specific capacitance of the composite reaches 170 F g⁻¹ in 1 M aqueous H₂SO₄ and 370 F g⁻¹ in 1M tetraethylammonium tetrafluoroborate in acetonitrile at a scan rate of 2 mV s⁻¹, both tested in symmetric 2-electrodes device. Moreover, in both cases the capacitance retention sustained at level <98% after 5000 cycles at a scan rate of 100 mV s⁻¹.

Acknowledgments: This work was financially supported by the National Science Center Grant no. 2019/33/N/ST5/00052 and grant no. 2019/35/B/ST5/01568.



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Resistive switching in transition metal dichalcogenides nanosheets exfoliated on conductive substrates

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P03

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Resistive switching effect is an ability of the material to reversibly change its conductivity after the electrical stimulation. One of the main desirable applications for this phenomenon is the technology of non-volatile computer memory, where distinguishable conductivity states are representing the logical states of the memory cell. Memory cells in resistive switching technology are simple MIM (metal/insulator/metal) structures, where switchable material is sandwiched between two metal electrodes. It is possible to change the resistance of an insulating material by polarizing the insulator with external electric field, which results in transition from a high resistivity state to a low resistivity state. By applying the same (unipolar resistive switching) or reverse (bipolar resistive switching) bias, the state of the device can be reset back to the high resistivity state. Resistive switching effect is now broadly studied in plenty of materials including transition metal dichalcogenides which are very promising candidates for such application due to their atomically thin structure and moderate band gap. Their general formula is MX_2 , where M is a transition metal and X is a chalcogen. Most widely studied transition metal dichalcogenide is an MoS_2 due to its environmental stability and low temperature chemical vapor deposition synthesis.

Our research is based on nanoscale investigation of MoS_2 nanosheets obtained by mechanical exfoliation using CAFM method (conductive probe atomic force microscopy) which allows us to examine local topography and conductivity changes after electrical stimulation.

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Study of liquid phase exfoliated graphene-like structures by Raman spectroscopy

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P04

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Graphene is a one of the most famous 2D material due to its remarkable physical properties. The application of graphene includes high frequency electronics, composite fillers, conductive coatings and many others. However, the production of large quantities of graphene is still limited by costs and process efficiency. In recent years a method for producing graphene by shear exfoliation in liquids has been developed [1]. This method could be potentially implemented in industrial production of graphene due to low defect density of graphene sheets. Moreover, the possibility to produce graphene by using kitchen mixer also has been reported [2]. In this work we are aiming to determine whether graphene exfoliation can be achieved simply by using kitchen mixer, instead of laboratory-scale shear mixers. Additionally, the impact of different mass ratio of surfactant – graphite on quality of graphene-like structures was investigated.

The graphene-like structures were produced by co-mixing 1 to 5 g of graphite powder and 1 to 5 g of Arabic gum in 100 ml of water. Arabic gum played a surfactant role, whereas shear mixing process was achieved by blending the mixture for 5 to 15 minutes. The mixture was then left to enable natural sedimentation. The samples were prepared by dropping of approximately 2.5 μL of the solution on glass slides and drying up. The samples were characterized by Raman spectroscopy and quality were determined basing on the position of D, G and 2D bands, characteristic for Raman spectra of carbon materials. Additionally, the intensity ratio of these bands: I_{2D}/I_G , I_D/I_G provided information about the number of graphene sheets in investigated samples.

The aim of this study is to determine the effectiveness of liquid phase exfoliation by kitchen blender in production of good quality multilayer graphene-like structures.

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On the electric properties of epitaxial carbon-enriched boron nitride structures

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Hexagonal boron nitride (h-BN) is a member of the 2D materials family, widely investigated for its potential use in optoelectronics in the deep UV range. Despite its exceptional properties, such as chemical stability, thermal conductivity and wide bandgap, its practical use is limited due to difficulties in obtaining high quality h-BN layers as well as the lack of ohmic contacts.

In this communication we explore the possibility of obtaining carbon-enriched boron nitride, grown using Metalorganic Vapor Phase Epitaxy (MOVPE), to manipulate the electrical properties of h-BN. By exchanging hydrogen for nitrogen as the carrier gas, otherwise reduced carbon radicals are introduced to the crystal structure of the grown material. The obtained samples were characterized using spectroscopic methods. Raman and infrared spectra as well as UV-Vis spectroscopy confirm the incorporation of carbon into our epitaxial layers.

Electrical measurements have also been performed on a specially prepared structure, manufactured by plasma etching and photolithography processes, using gold-palladium alloy as contact material. The results show a reduction in resistivity of several orders in magnitude in comparison to undoped h-BN.

The obtained results are very promising from the point of view of possible applications as contact or conductive layer in h-BN based devices.

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Exploring spin-orbit coupling in type-II Ising superconductors with the spin-mixing parameter

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P06

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Two-dimensional (2D) type-I Ising superconductors are very promising materials due to extraordinary high critical magnetic fields [1,2]. Spin-orbit coupling plays a crucial role in stabilizing superconductivity in these materials since it pins the electron spins to an out-of-plane direction. The same interaction is responsible for the formation of robust superconductivity in centrosymmetric type II Ising superconductors [3,2]. In the latter, the space inversion symmetry keeps spin up and spin down states in a band degenerate. This makes the characterization of spin-orbit coupling in the band structure more difficult than in non-centrosymmetric materials with spin split bands.

Here, we overcome this difficulty by calculating the spin mixing parameter b^2 . We employ first-principles calculations based on the density functional theory and calculate the spin-mixing parameter for a group of type-II Ising superconductors, such as NbTe₂ or TiSe₂, in a normal state [4,5]. Since the parameter b^2 can characterize the strength and anisotropy of spin-orbit coupling [6], we hope that our results will explain the contribution of different Fermi pockets to the formation of robust superconductivity in these materials.

Acknowledgements: The project is co-financed by the Polish National Agency for Academic Exchange.

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Synthesis and characterization of photosensitizer/graphene nanohybrids with potential application in cancer phototherapy

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Over the years, conventional therapies have failed to effectively treat cancer; as a direct consequence, the condition has become one of the major causes of mortality worldwide. Consequently, there is an urgent need to develop new medical therapies to improve the clinical prognosis for cancer patients. In recent years, photodynamic therapy (PDT) based on photosensitizers has gradually developed as one of the most promising non-invasive methods to combat tumors [1,2].

In PDT, cancerous cells are locally killed by reactive oxygen species (ROS) such as singlet oxygen 1O_2 produced by a photosensitizer (PS) under illumination and in the presence of oxygen. The broad applications of known photosensitizers are limited because of prolonged cutaneous photosensitivity, poor water solubility and inadequate selectivity [3,4]. Fortunately, the above mentioned problems may be gotten over by the emerging two dimensional layered materials (2DLM) with versatile properties [5]. 2DLM have a great prospects in application in PDT due to their large specific surface area and abundant functional groups that can serve as a PS carrier and in addition 2DLM may help to increase dispersibility of PS in a physiological environment [5–7]. In my work by functionalizing non-covalently two dye molecules (tetrakis (m-hydroxyphenyl)porphyrin and tetrakis (m-hydroxyphenyl)chlorin) to 2D-layered materials novel nanomaterials were constructed that were fully characterized by spectroscopic methods including determination of the yield of singlet oxygen generation.

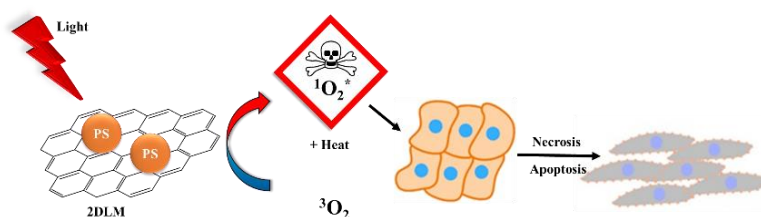


Fig. 1. Representation of a simple photothermal protocol for PS/2DLM materials.

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Interaction of light with anionic porphyrin/2D material hybrids

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P08

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 in e.g., photocatalysis, solar cells [1].

During photocatalytic processes, a common problem is low efficiency due to inefficient electron transfer. To obtain systems with higher charge separation efficiency, an interesting solution is to combine dye molecules with a graphene sheet, which acts 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 permanent charge separation, 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) or reduced graphene oxide (RGO) with the ultimate goal of obtaining material with photocatalytic activity.

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.

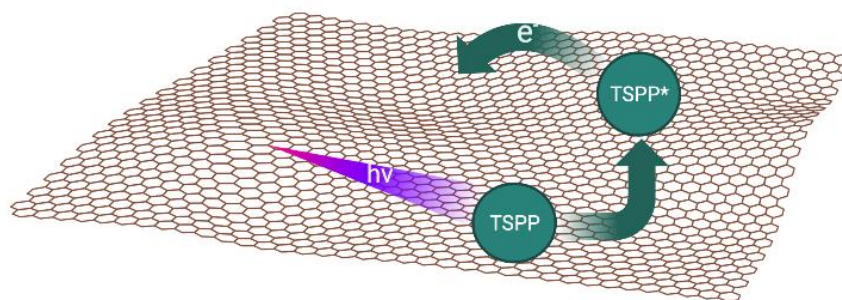


Fig. 1. Scheme for non-covalent functionalization of TSPP molecules on GO sheet.

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The influence of aminoalcohols on structure of ZnO thin films synthesized with sol-gel method

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P09

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The sol-gel method for producing high-quality structures has gained huge popularity because of the possibility of growing materials without specific equipment. One of the most frequently synthesized materials using the sol-gel method are nanocrystalline and amorphous oxides such as zinc oxide (ZnO) [1].

In preparing low-dimensional structures that would fulfill specific requirements, the control of the basal plane of crystallites, crystallite structures, or the appearance of the voids [Znaidi2010] is necessary. In the case of the ZnO layers, those parameters may depend on the nature of the precursor and its concentration in the solution, the solvent used, the solution concentration, the method of layer deposition, substrate, pre-and post-process annealing, etc. [1].

One of the critical factors in the formation of a layer and its homogeneity is additives. Additives may act as an additional precursor solvent, facilitate the complex formation, stabilize the sol, or help in forming thin films [2]. One of the substances that can participate in the formation of anionic ligands is amino alcohols, which allow control of the sol formation reaction [2, 3]. Since the aminoalcohols differ in boiling points and alkalinity, their selection may play a significant role in the dynamics of structure forming.

The poster comprehends the properties of ZnO layers grown using different aminoalcohols at different concentration rates. For a better comparison, the layers were grown on different substrates, which would give additional information about the behavior of the layers on a specific substrate. The research was conducted using monoethanolamine (MEA) and diethanolamine (DEA) in equal molar concentrations. The structure was estimated from morphology micrographs and Raman spectra for all samples. In addition, UV-vis absorption and photoluminescence were used to estimate structural defects.

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Construction of a Raman spectrometer for use in an inert gas atmosphere

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P10

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Raman spectroscopy is an experimental technique often used in the field of physics, chemistry and nanotechnology. It uses the Raman effect, the phenomenon of inelastic scattering of photons by the substance. Most commercial Raman spectrometers can only perform measurements in air. This is a serious disadvantage for many sensitive materials, as exposure to atmospheric conditions can modify the physicochemical properties of the surface or even transform one compound into another.

An example of such a chemical is solid rhenium heptoxide (Re_2O_7), the member of Transition-metal oxides (TMOs) group. Solid Re_2O_7 forms an orthorhombic unit cell of equal numbers of ReO_4 tetrahedra and ReO_6 octahedra, connected by corners and forming polymeric double layers with only oxygen-oxygen van der Waals contacts between the layers [1]. Dirhenium heptoxide is highly hygroscopic and decomposes into perrhenic acid (HReO_4) when exposed to moisture [2].

We present our development work on a unique mapping Raman spectrometer that enables characterization in the glove-box with an argon atmosphere. This integration allows the investigation of compounds and reactive materials under strictly controlled conditions. We show the advantage of this approach on the spectra of crystalline Re_2O_7 and the effect of exposure of the compound to the air for only seconds.

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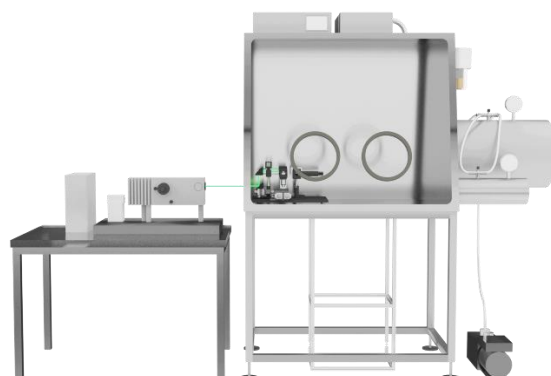


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The DFT calculation of the interactions between graphene and Td-WTe₂

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P11

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Graphene has opened the way to explore two-dimensional (2D) materials. The electron properties of 2D materials can differ significantly from their 3D counterparts. Scientists have recently become interested not so much in low-dimensional materials themselves, but more in their heterostructures. By overlaying two thin atomic layers of different substances, which are only connected through the interaction of van der Waals forces, a hybrid with more complex and unique properties is obtained.

In this paper, we will discuss the results of the study of the electronic properties of 2D hybrid materials based on graphene and Td-WTe₂. We will study in detail the phenomena occurring at the nanoscale and show the effect of interlayer interactions on the modification of the electronic properties of each component of the hybrid. Experimental data will be compared with calculations performed within the framework of density functional theory (DFT), which will enable us to comprehensively describe the physical phenomena occurring at the interface between the layers.

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

Graphene as oxidation protection layer for T_d tungsten (IV) telluride

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Layered 2D materials like graphene or transition metal dichalcogenides (TMDC) exhibit a diverse range of many unusual properties. Because of that, in recent years, they have been given a lot of attention and studies by both theoretical and experimental means. Unfortunately, the studies and usage of tungsten (IV) telluride (WTe₂) are restricted due to its rapid air degradation [1,2]. Thus, methods to preserve WTe₂ and other TMDCs are being researched. Some approaches have been already explored e.g., polymer encapsulation, coating with aluminium oxide or protection by inert 2D materials like hBN [1].

In our approach to protect WTe₂, we use a method of coating the TMDC with graphene that prevents its surface from air-induced degradation. So fabricated hybrids called van der Waals heterostructures were investigated by global and local characterisation methods. Bulk WTe₂ was chosen to create the heterostructure due to its extraordinary properties. It belongs to the group of type-II Weyl semimetals – a class of materials in which electrons behave as massless Weyl fermions with a well-distinguished chirality.

The deposition of graphene onto the WTe₂ surface is an effective way of protecting it from oxidation. It was checked using various techniques like scanning tunneling microscopy, low energy electron diffraction, Raman spectroscopy, X-ray photoelectron spectroscopy and angle-resolved photoelectron spectroscopy. Comprehensive investigations done by the above-mentioned techniques suggest not only the great effectiveness of surface protection by graphene overlayer but also the potential to use such heterostructures to study the interactions between TMDC and graphene, which is very important in fabricating modern low-dimensional heterostructures and devices.

This work was supported by the National Science Centre, Poland under project 2018/31/B/ST3/02450.

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Growth and oxidation of bismuthene on van der Waals substrates

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Bismuth belongs to the 15th group of the periodic table, with the electronic configuration $6s^26p^3$, and as a semi-metal it is the last non-radioactive element in the periodic table with unusual electronic properties.

These properties are of interest due to spin-orbital effects, surface and edge states [1]. Many quantum phenomena such as, for example, magnetoresistance, quantum size effects and recently also topologically protected edge states were firstly observed in bismuth. It was recently shown that bismuth can be grown in two-dimensional form and it is known as bismuthine [1,2]. It is extremely important to understand the growth and degradation processes of these new material.

We will present the properties and morphology of bismuth nanostructures grown epitaxially on a pyrolytic graphite (HOPG), as well as on insulating materials such as mica, on which the growth of bismuthene islands (2D bismuth with black phosphorus structure) can be observed.

We will focus on experimental research conducted using scanning tunneling microscopy and atomic force microscopy, thanks to which we were able to investigate the electronic and atomic structure of bismuth single layers. X-ray photoelectron spectroscopy was used to study and determine the chemical composition of the oxidized structures. Raman spectroscopy was used for further analysis of oxidized and metallic structures.

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The fast demagnetisation process in magnetic ultra-thin films by very short laser pulse of high power

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The process of the ultrafast laser-induced demagnetization in magnetic materials can be described by the Microscopic Three Temperature Model (M3TM) [1]. This approach is based on the simplified model of Hamiltonian describing free electrons, phonons and photons.

From the mathematical point of view finding the kinetics of the fast demagnetization process is a solution a set of three coupled differential equations that completely specify the magnetization dynamics m :

$$\begin{cases} C_e [T_e] \frac{dT_e}{dt} = \nabla_z (k \nabla_z T_e) + g_{ep} (T_p - T_e) \\ C_p \frac{dT_p}{dt} = g_{ep} (T_e - T_p) \\ \frac{dm}{dt} = Rm \frac{T_p}{T_c} (1 - m \coth(\frac{mT_c}{T_e})) \end{cases}$$

where ∇_z denotes differentiation with respect to z , and k is the electronic thermal conductivity, T_e, T_p represent temperature of electrons and phonons subsystems respectively. We suppose that these temperatures are different for electrons and phonons for a scale of time less than relaxation time of system, T_e, T_p and m are function z , the coordinate perpendicular to film surface. The values C_p and C_e are the values of phonon and electron specific heat respectively while T_c represents the Curie temperature.

In the case of ultra-thin magnetic films in numerical analysis it is necessary to consider the influence of the size effect on the basic parameters describing the sample such as a magnetization, the Curie temperature or the Fermi energy.

In order to describe the size effect and its influence on the results of calculations we use the concepts of magnetic equation of state for magnetic materials[2-4]. This idea allows us to consider the size effect in the relatively fast and easy method and allows us to avoid complicated time-consuming calculations based on the Density Functional Method(DFT).

The numerical results are interesting and show an influence of the size effect on the ultrafast demagnetization process in magnetic materials.

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- [2] T. Balcerzak, *J. Magn. Magn. Mater* **177-181**, 771 (1998).
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- [4] K. Warda, L. Wojtczak, *Acta Physica Polonica A* **131**, 878 (2017).

Investigations of exciton-trion and exciton-biexciton coupling in van der Waals hBN/WS₂/hBN heterostructures by upconversion photoluminescence excitation measurements

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The monolayer transition metal dichalcogenides (TMDCs) are unique systems to study electronic and phononic interactions as well as intra- and intervalley excitons and trions. These excitonic complexes are optically either active or inactive due to selection rules from spin or momentum conservation. In W-based materials the inverted order of the optically allowed and optically forbidden states in the K⁻/K⁺-valley results in a dark exciton band lying at lower energy than the bright band. Hence, their optical properties are determined by a manifold of bright and dark exciton states. The involved transitions positioned energetically below the bright direct exciton (X) have been identified as bright singlet and triplet trions, neutral and charged bright biexcitons, spin-forbidden dark excitons, dark trions and momentum-indirect dark excitons activated by scattering with defects or phonons. Recent works have demonstrated that upconversion (UPC) photoluminescence (PL) where, in contrast to the conventional PL, emission is detected

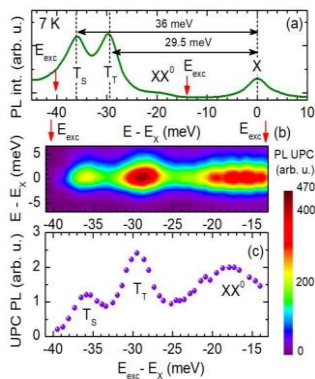


Fig. 1 (a) PL spectrum of WS₂ at 7 K. (b) Color map of the UPC PLE spectra. (c) Integrated UPC PL intensity of the exciton X as function of ΔE .

at energies above the excitation energy, is an alternative route to address the different excitonic species in TMDC monolayers [1, 2]. The excess energy required for the UPC process can be taken from either phonons or resident electrons in the monolayer; hence, the UPC PL provides information on both the energy spectra of the TMDC as well as the scattering mechanism related to exciton-electron, or exciton-phonon interaction. Here, we excite resonantly the UPC PL in hBN/WS₂/hBN heterostructures by tuning the laser energy between the T_S peak and the high-energy flank of the XX₀ peak, marked by the red arrows (Fig.1a). The UPC PLE spectra are depicted in the Fig. 1b by a color map which gives the X emission line as a function of the excitation energy E_{exc} detuned from E_x . The integration across the UPC PL energy range yields the dependence shown in the Fig.1c. It clearly exhibits three resonances at energy gains of 18, 29.5, and 36.0 meV. The first resonance matches the spectral positions of the biexciton XX₀ and further two correspond to the spin-triplet T_T and spin-singlet trion T_S, respectively. The revealing of the fine trion structure in the UPC PL sheds a new light on exciton-trion coupling in monolayer WS₂.

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Company information



Wyposażymy Twoje laboratorium

Działamy w obszarze nanoszenia powłok, modyfikacji powierzchni, mikroskopii świetlnej i profilometrii, badań mechanicznych w tym twardości, odporności na zarysowania czy zużycia.



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SPÓŁKA AKCYJNA

Dzięki wykorzystaniu prawdziwie przełomowych technologii z zakresu analizy materiałów w skali nano i mikro, jesteśmy w stanie dostarczać wysoce zaawansowane systemy badawcze wykorzystujące znane metody LEEM, PEEM, XPS, UPS, AFM, ARPES oraz ich kombinację. Sprowadzamy do Polski najlepsze i najbardziej obiecujące systemy ESCA działające jak w ultrawysokiej próżni tak i warunkach Near-Ambient Pressure. Zespół naszych inżynierów z wieloletnim doświadczeniem jest w stanie dobrać odpowiednią konfigurację sprzętu pomiarowego z uwzględnieniem wymagań konkretnej grupy badawczej lub pomóc w procesie rozbudowania już istniejącej aparatury.

Spółka Sygnis jest liderem również w dziedzinie mikro i nanofabrykacji. Oferowane przez nas hybrydowe systemy łączą metody zaawansowanego druku 3D, polimeryzację dwufotonową (2PP) oraz ablację materiału przy pomocy lasera o starannie dobranej długości fali. Pozwala to na wytwarzanie struktur z rozdzielczością do 200 nm i wysokim stopniem powtarzalności. Współpracujemy z największymi ośrodkami naukowymi w Polsce i Europie takimi jak Uniwersytet Łódzki, Narodowe Centrum Promieniowania Synchrotronowego Solaris, Uniwersytet Jagielloński w Krakowie, Uniwersytet Warszawski, etc.

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- analizatory: TN, TS, TOC, EOX, AOX, POX, NOX, CHNS (O), do oznaczania: azotu, siarki, chlorków, całkowitego węgla organicznego itd., o stężeniach od ppb do %,
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- kalorymetry, w tym najnowszy z zapłonem laserowym,
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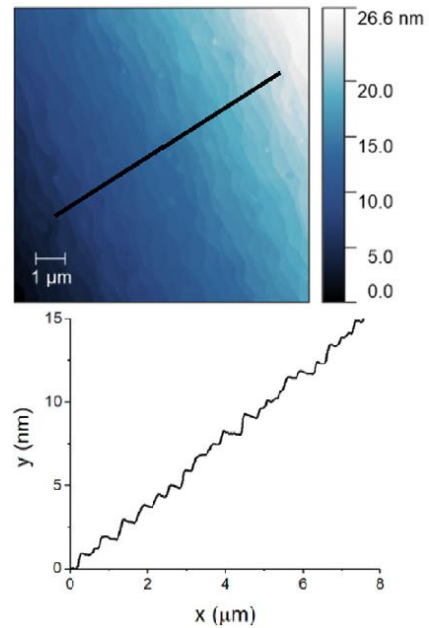
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BeeGraphene is the producer of high-quality graphene, grown directly on insulating, minimally step bunched silicon carbide wafers, with the lateral size of up to 2" (5cm).

After 6 years of research, BeeGraphene has developed a process which can solve the problems faced by the currently used production methods. It is based on a high-temperature graphitization of the surface of silicon carbide in ultra-high vacuum, with an external beam of silicon atoms directed at the surface. The material produced by BeeGraphene stands out not only due to the high quality of the surface, but also because of the highly ordered interface between graphene and silicon carbide.

Our method significantly limits step-bunching of silicon carbide during graphene growth (steps' height of around 1 nm), which results in the isotropic parameters, due to the undisturbed motion of electrons in every direction on the surface. The process we use in BeeGraphene is energy-efficient, environmentally-friendly and highly reproducible. Our company also offers few-layers graphene, with the ABC-stacking of the adjacent layers. What is best, our material is surprisingly affordable – please do not hesitate to contact us for a quotation.



AFM image of a bilayer graphene from BeeGraphene (top) and a line profile

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