## 2DQMS 2024



## - Book of Abstracts -

29<sup>th</sup> – 31<sup>st</sup> January 2024 Faculty of Physics Adam Mickiewicz University Poznań, Poland





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**Norway The Workshop is sponsored by the 2Dtronics consortium –** Polish-Norwegian research project financed from the Norwegian Financial Mechanism under the Basic Research Programme operated by the National Science Centre in Poland

## *NCN GRIEG: Spin and charge transport in low-dimensional novel quantum materials (2Dtronics) project No. 2019/34/H/ST3/00515*

*lead by prof. UAM Anna Dyrdał* (ISQI, Faculty of Physics Adam Mickiewicz University, Poznań, Poland) *in partnership with Dr Alireza Qaiumzadeh* (QuSpin/NTNU, Trondheim, Norway)

**2Dtronics** is focused on selected aspects of fundamental solid-state physics and magnetism, which may support the main concept of spintronics: efficient control of the spin state and its utilization on equal footing with quasiparticle charge. In principle, we focus on such subfields of spin electronics as spin-orbitronics, magnonics, and antiferromagnetic spintronics, where the symmetries and topological properties of the systems play an essential role. We investigate novel 2D materials that are promising platforms for phenomena where the topological nature of quasiparticle states plays an essential role and which allow for a variety of spin-to-charge interconversion effects.

We are combining the spin and valley degrees of freedom with the symmetries and topological properties of the system to describe and propose phenomena that enable us to work out new protocols for electronic and logic devices. Additionally, we investigate some emergent phenomena in low-dimensional quantum magnetic systems, which are important for both academic and application points of view. Another important question is the effect of many-body interactions in low-dimensional magnetic quantum materials.

In principle, we focus on theoretical models that reveal:

- topological invariant or topological charge,
- non-zero Berry curvature dipole,
- desired symmetry properties,
- experimentally tunable parameters.

More details You can find at the webpage <u>https://2dtronics.amu.edu.pl</u>





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2Dtronics Team, Będlewo 2023

29<sup>th</sup> January 2024

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Opening	
14:00 - 14:15	Anna Dyrdał
Session 1	
14:15 - 14:45	Topological crystalline insulators – from crystal facets with atomic steps to layered heterostructures and nanowires Tomasz Story Institute of Physics, Polish Academy of Sciences, Warsaw, Poland & International Research Centre MAGTOP, Institute of Physics Polish Academy of Sciences, Warsaw, Poland
14:45 - 15:15	Nontrivial topological phases in superconducting nanostructures Tadeusz Domański Institute of Physics, M. Curie-Skłodowska University, Lublin, Poland
15:15 - 15:30	Topological insulator and quantum memory Levan Chotorlishvili Department of Physics and Medical Engineering, Rzeszów University of Technology, Poland

### COFFEE BREAK 15:30 - 16:00

Session 2	
16:00 - 16:30	Bosonic fluctuations in 2D materials Artur Ernst Johannes Kepler University of Linz, Austria & Max Planck Institute of Microstructure Physics Halle, Germany
16:30 - 17:00	In-plane Magnetic Skyrmion Valve Made of 90° Pinned Magnetic Domain Walls Pavel Baláž FZU-Institute of Physics of the Czech Academy of Sciences, Prague, Czech Republic
17:00 - 17:30	Tailoring magnetic properties of Co/Ni bilayers by plasma oxidation Piotr Kuświk Institute of Molecular Physics, Polish Academy of Sciences, Poznań, Poland
D 0	45.00 40.00

POSTER SESSION 17:30 - 19:30

Pavel Baláž, Michał Inglot, Maciej Kalka, Piotr Pigoń, Sakineh Vosoughi-nia, Amir N. Zarezad, Anna Krzyżewska, Kateryna Boboshko, Izabella Wojciechowska, Stefan Stagraczyński

30th January 2024

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## SESSION 3

10:00 - 10:30	A tale of quantum anomalous Hall effect and parity anomaly Ewelina Hankiewicz University of Würzburg, Am Hubland, Germany
10:30 - 11:00	Two-dimensional materials as a platform for spin-orbit torque memories Jose Hugo Garcia Aguilar Catalan Institute of Nanoscience and Nanotechnology, Barcelona, Spain
11:00 - 11:30	Superconducting spintronics with interfacial spin-orbit coupling and symmetry filtering César González-Ruano Universidad Autónoma de Madrid. Spain

## COFFEE BREAK 11:30 - 12:00

## SESSION 4

12:00 - 12:30	Spin-orbitronics in chiral crystals Jagoda Sławińska Zernike Institute for Advanced Materials, University of Groningen, The Netherlands
12:30 - 13:00	Microscopic theory of the spin Hall effect in twisted van der Waals heterostructures Aires Ferreira School of Physics, Engineering and Technology and York Centre for Quantum Technologies, University of York, United Kingdom
13:00 - 13:30	Charge density wave-controlled effects in graphene on transition metal dichalcogenides: NbS <sub>2</sub> and TaS <sub>2</sub> Karol Szałowski Department of Solid State, Faculty of Physics and Applied Informatics, University of Łódź, Poland

## LUNCH 13:30 - 15:00

Session 5	2DTRONICS SESSION
15:00 - 15:15	Introduction to the 2Dtronics session Anna Dyrdał
15:15 - 15:45	Electrically Controlled Crossed Andreev Reflection in Two-Dimensional Antiferromagnets Alireza Qaiumzadeh Center for Quantum Spintronics, Norwegian University of Science and Technology, Trondheim, Norway

15:45 - 16:00	Topological Hall effects due to Skyrmions in Antiferromagnets Amir N. Zarezad ISQI, Faculty of Physics, Adam Mickiewicz University, Poznań, Poland
16:00 - 16:15	Magnons in the VX2 (X=S, Se, Te) monolayer and bilayer TMD systems Wojciech Rudziński ISQI, Faculty of Physics, Adam Mickiewicz University, Poznań, Poland
16:15 - 16:30	Magnetic properties of Vanadium-based Transition metal dichalcogenides Mirali Jafari ISQI, Faculty of Physics, Adam Mickiewicz University, Poznań, Poland
16:30 - 16:45	Spin-orbit coupling driven phenomena in twisted graphene on transition metal dichalcogenides Izabella Wojciechowska ISQI, Faculty of Physics, Adam Mickiewicz University, Poznań, Poland

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## COFFEE BREAK 16:45 – 17:15

17:15 - 17:30	Magnetism of CrX₃ hexagonal layers win the atomistic spin dynamics <mark>Stefan Stagraczyński</mark> ISQI, Faculty of Physics, Adam Mickiewicz University, Poznań, Poland
17:30 - 17:45	Topological magnon gap engineering in 2D van der Waals CrI3 ferromagnets Verena Brehm Center for Quantum Spintronics, Norwegian University of Science and Technology, Trondheim, Norway
17:45 - 18:00	Non-linear anomalous Hall effect in a 2DEG with different forms of Rashba spin-orbit interaction Anna Krzyżewska ISQI, Faculty of Physics, Adam Mickiewicz University, Poznań, Poland
18:00 - 18:15	Bilinear magnetoresistance and planar Hall effect in topological insulators: interplay of scattering on spin-orbital impurities and non-equilibrium spin polarization Kateryna Boboshko ISQI, Faculty of Physics, Adam Mickiewicz University, Poznań, Poland

Conference Dinner 18:30 - ...

31<sup>st</sup> January 2024

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## SESSION 6

10:00 - 10:30	Fermi level control in topological insulators Marek Przybylski Academic Centre for Materials and Nanotechnology, AGH University of Krakow, Poland
10:30 - 11:00	Connection between the semiconductor-superconductor transition and the spin-polarized superconducting phase in the honeycomb lattice Agnieszka Cichy ISQI, Faculty of Physics, Adam Mickiewicz University in Poznań, Poland
11:00 - 11:30	Topological phase transition in 1D quantum spin system <b>Piotr Tomczak</b> <i>IF, Faculty of Physics, Adam Mickiewicz University, Poznań, Poland</i>

#### COFFEE BREAK 11:30 - 12:00

SESSION 7

12:00 - 12:30	Compact localised states in magnonics Jarosław W. Kłos ISQI, Faculty of Physics, Adam Mickiewicz University in Poznań, Poland
12:30 - 13:00	Magnetization dynamics in two-dimensional ferromagnets Witold Skowroński Institute of Electronics, AGH University of Krakow, Poland & CIC NanoGUNE BRTA, San Sebastián, Spain
13:00 - 13:15	A First-Principles Study of Magnetic Properties and Structural Phase Transitions in Ultra-Thin Fe Films Justyna Rychły-Gruszecka Institute of Molecular Physics, Polish Academy of Sciences, Poznań, Poland
13:15 - 13:30	Impact of ion bombardment on ferrimagnetic Tb/Co multilayers using different ion species Daniel Kiphart Institute of Molecular Physics, Polish Academy of Sciences, Poznań, Poland

CLOSING 13:30

LUNCH 13:30 - 15:00

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## January 29th

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Sessions 1–2

## Topological crystalline insulators – from crystal facets with atomic steps to layered heterostructures and nanowires

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#### T. Story<sup>1,2</sup>

 <sup>1</sup> Institute of Physics, Polish Academy of Sciences, al. Lotników 32/46, 02-668 Warsaw, Poland
 <sup>2</sup> International Research Centre MAGTOP, Institute of Physics Polish Academy of Sciences, al. Lotników 32/46, 02-668 Warsaw, Poland

Topological crystalline insulators (TCI) constitute a class of topological materials exhibiting surface (2D) and edge (1D) electronic states with Dirac-like linear dispersion and spin-momentum locking. Protected by mirror-plane symmetry, TCI 2D states are observed in SnTe, Pb<sub>1-x</sub>Sn<sub>x</sub>Te and Pb<sub>1-x</sub>Sn<sub>x</sub>Se IV-VI semiconductors at (100) and (111) facets of single bulk crystals as well as epitaxial layers [1-3]. Experimental techniques applied so far to study these materials cover angle- and spin-resolved photoemission (ARPES), scanning tunneling spectroscopy (STM/STS) as well as magneto-transport and magneto-optical measurements.

New type of 1D topological states are observed at the edges along atomic steps (of 1, 3, 5 monolayer height) at (100) TCI surface [1,3] as superimposed on regular TCi surface states. I will discuss new observations concerning the coupling of 1D states located along nearby edges and the influence of electron-electron interactions on the local density of states at atomic steps in the surface doping controlled regime of resonant position of the Fermi level with respect to the Dirac point [3].

New developments in TCI materials resulted in successful growth of IV-VI topological nanowires, including cubic SnTe [4], core-shell GaAs/Pb<sub>1-x</sub>Sn<sub>x</sub>Te [5] and Pb<sub>1-x</sub>Sn<sub>x</sub>Te of both cubic and (unusual) pentagonal cross-section symmetry (assembly of cubic sections with twin crystal boundaries). I will address the important point of experimental verification of various theoretical predictions, including thickness controlled topological transitions and hinge or corned states hosting zero-energy modes in nanowires [6-8].

- [1] P. Sessi et al., Science 354, 1209 (2016).
- [2] B. Turowski et al., Appl. Sur. Sci. 610, 155434 (2023).
- [3] G. Wagner et al., Nano Lett. 23, 2476 (2023).
- [4] J. Sadowski et al., Nanoscale 10, 20772 (2018).
- [5] S. Dad et al., Scientific Reports 14, 589 (2024).
- [6] G. Hussain et al., arXiv: 2401.03455.
- [7] N. M. Nguyen, W. Brzezicki, T. Hyart, Phys. Rev. B 105, 075310 (2022).
- [8] S. Samadi, R. Rechciński, R. Buczko, Phys. Rev. B 107, 205401 (2023).

### Nontrivial topological phases in superconducting nanostructures

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#### T. Domański<sup>1</sup> and M. Maśka<sup>2</sup>, and I. Weymann<sup>3</sup>

 <sup>1</sup> Institute of Physics, M. Curie-Skłodowska University, 20-031 Lublin, Poland
 <sup>2</sup> Institute of Theoretical Physics, Wrocław University of Science and Technology, 50-370 Wrocław, Poland
 <sup>3</sup> Institute of Spintronics and Quantum Information, Faculty of Physics, A. Mickiewicz University, 61-614 Poznań, Poland

Magnetism and superconductivity have been often regarded to be competing phenomena, as e.g. manifested by the Meissner effect. In nanostructures, however, magnetic textures combined with electron pairing could cooperate, giving rise to qualitatively new states of matter with exotic boundary quasiparticles. Various topologically nontrivial phases emerge when low dimensional magnetic structures are embedded into conventional bulk superconductors, inducing the triplet pairing. Under such circumstances there appear the Majorana quasiparticles confined on internal defects in p-wave superconductors, localized at the ends of magnetic chains [1] and ladders [2], at interfaces of the planar Josephson junctions [3] and along the edges/hinges of higherdimensional topological superconductors. Intensive theoretical and experimental studies are motivated by fractional character of such zero-energy modes, which are promising candidates for constructing stable qubits (immune to external perturbations due to topological protection) and perspectives of quantum computations (by virtue of their non-Abelian character). Under extreme conditions the Majorana quasiparticles can be realized even in the minimalistic two-site Kitaev chain [4]. We shall overview recent proposals concerning topological phases and discuss methods for detecting the Majorana-type quasiparticles, including the quantum dot nonohybrid structures under equilibrium [5] and nonequilibrium conditions [6].

[1] M. M. Maśka, A. Gorczyca-Goraj, J. Tworzydło, T. Domański, Phys. Rev. B 95, 045429 (2017).

[2] M. M. Maśka, N. Sedlmayr, A. Kobiałka, T. Domański, Phys. Rev. B 103, 235419 (2021).

[3] Sz. Głodzik, N. Sedlmayr, T. Domański, Phys. Rev. B 102, 085411 (2020).

### **Topological insulator and quantum memory**

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## M. Kulig<sup>1</sup>, P. Kurashvili<sup>2</sup>, C. Jasiukiewicz<sup>1</sup>, M. Inglot<sup>1</sup>, S. Wolski<sup>1</sup>, S. Stagraczyński<sup>3</sup>, T. Masłowski<sup>1</sup>, T. Szczepański<sup>1</sup>, R. Stagraczyński<sup>1</sup>, V. K. Dugaev<sup>1</sup>, and <u>L. Chotorlishvili<sup>1</sup></u>

<sup>1</sup> Department of Physics and Medical Engineering, Rzeszów University of Technology, 35-959 Rzeszów, Poland <sup>2</sup> National Centre for Nuclear Research, Warsaw 00-681, Poland

<sup>3</sup> Institute of Spintronics and Quantum Information, Faculty of Physics, Adam Mickiewicz University, Poland

Measurements performed on quantum systems are too specific. Unlike their classical counterparts, quantum measurements can be invasive and destroy the state of interest. Besides, quantumness limits the accuracy of measurements performed on quantum systems. Uncertainty relations define the universal accuracy limit of the quantum measurements. Relatively recently, it was discovered that quantum correlations and quantum memory might reduce the uncertainty of quantum measurements. In this paper, we study two different types of measurements performed on the topological system. Namely, we discuss measurements performed on the spin operators and measurements performed on the canonical pair of operators: momentum and coordinate. We quantify the spin operator's measurements through the entropic measures of uncertainty and exploit the concept of quantum memory. In contrast, for the momentum and coordinate operators, we exploit the improved uncertainty relations. We discover that quantum memory reduces the uncertainties of spin measurements. On the other hand, we prove that the uncertainties in the measurements of the coordinate and momentum operators depend on the value of the momentum and are substantially enhanced at small distances between itinerant and localized electrons. We suggest an indirect measurement scheme for the momentum and coordinate operators through the spin operator. Due to the factor of quantum memory, such indirect measurements in topological insulators have smaller uncertainties than direct measurements.

M. Kulig, P. Kurashvili, C. Jasiukiewicz, M. Inglot, S. Wolski, S. Stagraczyński, T. Masłowski, T. Szczepański, R. Stagraczyński, V. K. Dugaev, and L. Chotorlishvili, *Phys. Rev. B* 108, 134411 (2023).
 S. Wolski, M. Inglot, C. Jasiukiewicz, K. A. Kouzakov, T. Masłowski, T. Szczepański, S. Stagraczyński, R. Stagraczyński, V. K. Dugaev, and L. Chotorlishvili, *Phys. Rev. B* 106, 224418 (2022).
 P. Kurashvili, L. Chotorlishvili, *Journal of Physics A: Mathematical and Theoretical* 55, 495303 (2022).
 P. Kurashvili, L. Chotorlishvili, K. A. Kouzakov, A. G. Tevzadze, and A. I. Studenikin, *Phys. Rev. D* 103, 036011 (2021).

### **Bosonic fluctuations in 2D materials**

#### A. Ernst<sup>1,2</sup>

<sup>1</sup> Johannes Kepler University of Linz, Altbergerstraße 69, 4040 Linz, Austria <sup>2</sup> Max Planck Institute of Microstructure Physics, Weinberg 2, 06120 Halle (Saale), Germany

Electron-boson interactions such as charge, spin, and orbital fluctuations can significantly affect electronic, magnetic and transport properties in many systems. These bosonic fluctuations can be responsible for many interesting phenomena such as superconductivity, charge and spin density waves, suppressed or enhanced magnetism, exotic optical transitions etc. In my talk I present our recent studies on bosonic fluctuations in 2D materials, focusing on lattice and spin fluctuations in some 2D magnets. First, I introduce our first-principles approach for treatment of spin fluctuations in ordered and disordered materials [1]. This approach is based a many-body perturbation theory we approximate numerically complex quantities with quantities from timedependent density functional theory. As next, I discuss our recent studies on spin fluctuations in CeCo<sub>2</sub>P<sub>2</sub> and LaCo<sub>2</sub>P<sub>2</sub> [2,3]. These materials consist of ferromagnetic layers, which are weakly coupled together via ferro- or antiferromagnetic interaction. Electron-magnon interaction induces a strong renormalization of electronic structure in these materials. In its turn, a specific electronic structure ensures for long living spin waves. As next, I present our recent studies of light-driven topological and magnetic transitions in bilayer CrI<sub>3</sub> and in thin layer antiferromagnets MnBi<sub>2</sub>Te<sub>4</sub> and MnSb<sub>2</sub>Te<sub>4</sub>. Analyzing lattice vibrations driven via optical excitations we found specific phonon modes, which can lead to magnetization switch in these 2D materials [4,5].

- [1] S. Paischer et al., Phys. Rev. B 107, 134410 (2023).
- [2] G. Poelchen et al., Nature Communications 14, 5422 (2023).
- [3] D. Yu. Usachov et al., to be published (2024).
- [4] M. Rodriguez-Vega et al., Phys. Rev. B 102, 081117(R) (2020).
- [5] M. Rodriguez-Vega et al., Phys. Chem. Lett. 13, 4152 (2022).

Acknowledgements: Österreichischer Wissenschaftsfonds (FWF).

## In-plane Magnetic Skyrmion Valve Made of 90° Pinned Magnetic Domain Walls

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#### P. Baláž<sup>1</sup>

<sup>1</sup> FZU-Institute of Physics of the Czech Academy of Sciences, Na Slovance 1999/2, 182 21 Prague 8, Czech Republic

Magnetic skyrmions are small spherical whirls in the vector field of magnetization known for their high stability. Typically, they can be found in thin films or magnetic multilayers featuring Dzyaloshinskii-Moriya interaction in combination with perpendicular magnetic anisotropy. Recently, number of theoretical studies and numerical simulations have shown a possibility of existence of in-plane skyrmions in magnetic thin layers with in-plane easy-axis magnetic anisotropy and interfacial DMI [1]. These topological defects known as in-plane skyrmions, or sometimes as asymmetric skyrmions [2], or bimerons substantially differ from their out-of-plane twins. Unlike skyrmions in systems with perpendicular magnetic anisotropy, the in-plane skyrmions of both topological charges ( $Q=\pm1$ ) can simultaneously exist in the same magnetic domain.



Importantly, in-plane magnetic skyrmions can interact with planar magnetic textures, like 90° pinned magnetic domain walls (DWs), which are stable in hybrid multilayers consisted of ferromagnetic and ferroelectric layers [3,4]. Here, we show that a charged 90° DW can act as a topological-charge-selective filter of in-plane magnetic skyrmions. Namely, skyrmions crossing a 90° DW can pass or be annihilated according to their skyrmion charge (Fig: left panel). This effect is caused by out-of-plane magnetization in the DW, which is induced by the presence of DMI. Combining two magnetic DWs, we suggest an in-plane skyrmion valve able to control the flow of skyrmion topological charge [5] (Fig: right panel).

[1] K.-W. Moon, J. Yoon, C. Kim, and C. Hwang, Phys. Rev. Appl. 12, 064054 (2019).

[2] A. O. Leonov, and I. Kézsmárki, Phys. Rev. B 96, 014423 (2017).

[3] B. V. de Wiele, S. J. Hämäläinen, P. Baláž, F. Montoncello, and S. van Dijken, Sci. Rep. 6, 1 (2016).

[4] P. Baláž, S. J. Hämäläinen, and S. van Dijken, Phys. Rev. B 98, 064417 (2018).

[5] P. Baláž, Phys. Rev. Appl. 17, 044031 (2022).

Acknowledgements: This work is supported by the Czech Science Foundation (Project No. 19-28594X).

### Tailoring magnetic properties of Co/Ni bilayers by plasma oxidation

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#### M. Matczak<sup>1</sup>, B. Anastaziak<sup>1</sup>, M. Kowacz<sup>1</sup>, M. Urbaniak<sup>1</sup>, D. Kiphart<sup>1</sup>, F. Stobiecki<sup>1</sup>, A. Mandziak<sup>2</sup>, E. Madej<sup>3</sup>, D. Wilgocka-Ślęzak<sup>3</sup>, <u>P. Kuświk<sup>1</sup></u>

 <sup>1</sup> Institute of Molecular Physics, Polish Academy of Sciences, ul. M. Smoluchowskiego 17, 60-179, Poznań, Poland
 <sup>2</sup> Solaris National Synchrotron Radiation Centre, Jagiellonian University, ul. Czerwone Maki 98, 30-392 Kraków, Poland
 <sup>3</sup> Jerzy Haber Institute of Catalysis and Surface Chemistry Polish Academy of Sciences, ul. Niezapominajek 8, 30-239, Kraków, Poland

Currently, Co/Ni layered systems are intensively studied because they offer tuneable perpendicular magnetic anisotropy (PMA) together with low Gilbert damping and high spin polarization [1]. Moreover, Co/Ni covered by heavy metal or oxide layers shows Dzyaloshinskii-Moriya interaction (DMI) [2,3], which is important for perspective application in memories based on skyrmion motion. Recently, it was also shown that exchange-bias (EB) coupling can stabilize skyrmions at room temperature without an external magnetic field [4]. Therefore, the materials combining in themselves EB, DMI, and PMA are crucial for skyrmion-based applications.

For this reason, we focused on Co/Ni bilayers modified by plasma oxidation (PO). We show that the PMA can be tailored by a variation of oxidation time [5]. We attribute this effect not only to the reduction of Ni layer thickness due to oxidation but also to the change of EB coupling between antiferromagnetic (NiO) and ferromagnetic (Co/Ni) sublayers. This enhances the surface contribution to the effective anisotropy, favouring the perpendicular orientation of the Co/Ni [6]. The presence of a NiO layer after oxidation also induces DMI, which stabilizes right-handed chirality in domain walls. Moreover, oxidation can be performed locally, which allows 2D structures to be fabricated with different combinations of magnetic properties in the areas modified by plasma oxidation and in the areas protected against oxidation. All of these results show that Co/Ni systems subjected to plasma oxidation are promising materials for novel applications in spintronics and magnonics.

- [1] S. Andrieu, et al., Phys. Rev. Materials. 2, 064410, (2018).
- [2] G. Chen, et al., Nature Com., 4, 2671, (2013).
- [3] G. Chen, et al., Sci. Adv., 6, eaba4924, (2020).
- [4] G. Yu, et al., Nano Letters 18, 980 (2018).
- [5] B. Anastaziak, et al., Phys. Status Solidi RRL, 16, 2100450 (2022).
- [6] B. Anastaziak, et al, Scientific Reports 12, 22060 (2022).

Acknowledgements: This work was supported by the National Science Centre, Poland under OPUS 17 funding (Grant No. 2019/33/B/ST5/02013).

2D Quantum Materials for Spintronics, 2DQMS 29th – 31st January 2024 Poznań, Poland CONCERNMENT (CARACTER CONCERNMENT)

## January 30<sup>th</sup>

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Sessions 3-5

## A tale of quantum anomalous Hall effect and parity anomaly

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#### Ewelina M. Hankiewicz<sup>1</sup>

<sup>1</sup> University of Wurzburg, Am Hubland, Wuerzburg, Germany

Recent theoretical and experimental advances allow for an observation of signatures of quantum anomalies in non-interacting condensed matter systems. Quantum anomalies violate one of the classical symmetries and bridge between condensed matter and high-energy physics.

In this talk, I first introduce briefly topological states of matter and quantum anomalies. The possibility of observation of signatures of the parity anomaly (failure of the existence of single Dirac fermion in two spatial dimensions characterized by broken parity symmetry) in Dirac-like materials [1,2] is especially interesting. Using effective field theories and analyzing band structures, we predicted that quantum anomalous Hall (QAH) insulators survives in external out-of-plane magnetic fields (orbital fields) [2]. Furthermore, we showed that this effect is related to the parity anomaly. This leads in orbital fields to counter-propagating QAH and quantum Hall (QH) edge states without any electron-electron interactions (see Fig.1) and a new structure of quantum Hall plateaus [2]. Indeed, we showed together with experimentalists a novel transition from -1 to 1 Hall plateau in disordered (Hg,Mn)Te, quantum wells caused by scattering processes between counter-propagating quantum Hall and QAH edge states related to the parity anomaly [3]. Our model can be extended easily to any three-dimensional topological insulators (TIs) or magnetic 3D TIs with odd numbers of surface states involved in transport [4].

[1] F. D. M. Haldane, Phys. Rev. Lett. 61, 2015 (1988).

2] J. Böttcher, C. Tutschku, L. W. Molenkamp, and E. M. Hankiewicz, *Phys. Rev. Lett.* 123, 226602 (2019);
C. Tutschku, F. S. Nogueira, C. Northe, J. van den Brink, and E. M. Hankiewicz, *Phys. Rev. B* 102, 205407 (2020);
C. Tutschku, J. Böttcher, R. Meyer, and E. M. Hankiewicz, *Phys. Rev. Research* 2, 033193 (2020).
[3] S. Shamim, P. Shekhar, W. Beugeling, J. Böttcher, A. Budewitz, J.-Benedikt Mayer, L. Lunczer, E. M. Hankiewicz, H. Buhmann, L. W. Molenkamp, *Nat. Commun.* 13, Article number: 2682 (2022).
[4] L.Wang, W. Beugeling,...,E. M. Hankiewicz and L.W. Molenkamp, *submitted to Advanced Materials* (2023).

### Two-dimensional materials as a platform for spin-orbit torque memories

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#### Jose H. Garcia<sup>1</sup>, Joaquin Medina Dueñas<sup>1,2</sup>, and Stephan Roche<sup>1,2,3</sup>

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

<sup>2</sup> Department of Physics, Universitat Autónoma de Barcelona (UAB), Campus UAB, Bellaterra, 08193 Barcelona, Spain

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The emergence of two-dimensional materials has paved the way for numerous applications across a wide range of fields, from nanomedicine to advanced materials. Particularly noteworthy is their large surface-to-volume ratio and inherent stability, making them ideal for interface-based technologies. Spin-orbit coupling, a relativistic effect, links electron spins with their motion, offering the potential for electrical control over the spin properties of matter. A key application of spin-orbit coupling is spin-orbit torque, which arises from the disruption of inversion symmetries and is particularly pronounced at material interfaces. This phenomenon enables the generation of a non-equilibrium spin density, capable of interacting with a magnetic memory to induce magnetic oscillations and switching. The dynamics induced by this torque are influenced by the system's symmetries and chemical composition. In this talk, we will explore the current advancements in spin-orbit torque within two-dimensional systems, examining why these structures are crucial in addressing long-standing challenges and how Dirac materials may present opportunities for optimized spin-orbit torques.

[1] J. M. Dueñas, J. H. García, S. Roche, arXiv:2310.06447 (2023).

[2] H. Kurebayashi, J. H. Garcia, S. Khan, J. Sinova, S. Roche, Nat. Rev. Phys. 4, 150 (2022).

# Superconducting spintronics with interfacial spin-orbit coupling and symmetry filtering

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#### <u>C. González-Ruano</u><sup>1</sup>, D. Caso<sup>1</sup>, P. Tuero<sup>1</sup>, L. G. Johnsen<sup>2</sup>, J. A. Ouassou<sup>2</sup>, C. Tiusan<sup>3</sup>, Y. Lu<sup>4</sup>, I. Zutic<sup>5</sup>, J. Linder<sup>2</sup> and F. G. Aliev<sup>1</sup>

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Generation and control over long-range triplet (LRT) Cooper pairs is a key milestone for applications in superconducting spintronics. It has been commonly expected that this requires complex ferromagnetic multilayers, non-collinear magnetization or half-metals. Over the last years, we have developed a novel type of superconducting spintronics heterostructures, consisting of fully epitaxial ferromagnet/superconductor (F/S) junctions with interfacial spin-orbit coupling (SOC) and symmetry filtering [1-4].

First, we observed a thousand-fold increase in tunnelling anisotropic magnetoresistance below the superconductor critical temperature, which supports SOC-induced LRT formation depending on the magnetic configuration of the F layer [1]. Then, by using F/F/S junctions, we demonstrated the converse effect: the transformation of the magneto-crystalline anisotropy of the F layer driven by superconductivity [2,3], which would allow for an active control of magnetic anisotropies in spintronic systems. We have also presented experimental evidence illustrating the controllability of the superconducting thermoelectric effects in the same F/F/S system, through the manipulation of the magnetic alignment of the ferromagnetic electrodes [4]. This directly addresses the main challenge associated with conventional thermoelectric devices: their limited efficiency and versatility, which has hindered wide-spread adoption. Our current studies focus on the different mechanisms of LRT generation by studying periodic conductance anomalies in the F/F/S junctions, which arise due to quasiparticle interference within the F layer interfacing the superconductor. These features exhibit strong insensitivity to high magnetic fields while presenting an anisotropic low-field response, suggesting the potential to distinguish between the effects of SOC and magnetic textures in the generation of LRT Cooper pairs [5].

Our work establishes for the first time the important role of both spin-orbit coupling and symmetry filtering in fully epitaxial superconducting spintronics, paving the way for a broad range of potential next-generation technologies such as thermoelectric generators and cryogenic memories.

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## **Spin-orbitronics in chiral crystals**

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Chiral materials, similarly to human hands, have distinguishable right-handed and left-handed enantiomers which may respond differently to external stimuli, such as electric fields. One of the most intriguing aspects of chirality is its impact on charge-to-spin conversion (CSC) which is responsible for transforming electric currents into spin signals. Interestingly, chiral systems often outperform non-chiral ones in terms of conversion efficiency and facilitate long-range spin transport, which makes them relevant for both fundamental and applied physics.

In this talk, I will focus on chiral crystals that showcase chirality-dependent CSC and long-range spin transport. For instance, in Te, FeSi and TaSi<sub>2</sub>, electric currents induce an accumulation of spins that align either parallel or anti-parallel to them, resembling the phenomenon of chirality-induced spin selectivity (CISS) found in molecules. These materials not only exhibit efficient CSC, but also possess electronic structure features that may contribute to very long spin lifetimes.

In the second part of the talk, I will discuss the potential of chirality-dependent CSC and spin transport in two-dimensional (2D) chiral crystals. These materials can be realized as thin films of three-dimensional materials, such as Te whose 2D version is called tellurene. Another possibility is the creation of artificial chiral materials made of twisted van der Waals (vdW) crystals, where twisting in two opposite directions generates left- and right-handed versions of the same system. The abundance of possibilities opens up new perspectives for spintronics devices.

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## Microscopic theory of the spin Hall effect in twisted van der Waals heterostructures

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The goal of graphene-based spin-valve experiments is to measure a non-local resistance due the inverse spin Hall and spin galvanic effects upon injection of a spin current, with the aim of unravelling the physics of these spin-charge conversion processes [1]. We develop a microscopic theory of the spin Hall effect for twisted graphene/transition metal dichalcogenide bilayers within the diffusive limit, reflective of recent spin valve experiments, to obtain the total spin Hall response. Employing a self-consistent treatment of disorder, we obtain analytic formulae for the spin Hall conductivity in the weak scattering limit and study its dependence on both twist angle and spin-orbit coupling (SOC) strength. As an application of the theory, we make predictions about the SOC magnitudes needed to observe the spin Hall effect [2]. We obtain average SOC strengths and associated non-local resistances in good agreement with experimental observation and supporting recent claims about the giant magnitude of proximity-induced SOC within these systems [3].

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## Charge density wave-controlled effects in graphene on transition metal dichalcogenides: NbS<sub>2</sub> and TaS<sub>2</sub>

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Van der Waals heterostructures provide a platform to tailor graphene properties owing to proximity effects [1]. Charge density wave degree of freedom offers an interesting tool to reversibly manipulate the electronic structure of van der Waals heterostructures composed of graphene and selected transition metal dichalcogenide. Within this class, 1T polytypes of TaS<sub>2</sub> and NbS<sub>2</sub> can be mentioned, developing a low-temperature charge density wave with  $\sqrt{13} \times \sqrt{13}$  reconstruction.



Fig. Band structure for monolayer  $1T-NbS_2$ /graphene heterostructure supercell in the absence of charge density wave and the zoomed graphene band structure in the vicinity of K point.

In the paper we discuss DFT calculations-based predictions of proximity effects in graphene band structure emerging in heterostructures with TaS2 [2] and NbS2 and controllable with charge density wave ordering. The external electric field is demonstrated to be another useful factor influencing the band structure. The results are interpreted using symmetry-based tight-binding Hamiltonians [2]. Special emphasis is put on proximity-induced Rashba spin-orbit coupling parametrized by characteristic energy and tuneable angle (inducing possible anisotropic Rashba-Edelstein effect).

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## Electrically Controlled Crossed Andreev Reflection in Two-Dimensional Antiferromagnets

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In this talk, I first review our recent theoretical works on antiferromagnetic-superconductor junctions in both clean and dirty limits [1-4]. Next, I show how these junctions can be used to generate a perfect crossed Andreev reflection (CAR) and hence a novel Cooper pair splitter to generate entangled pairs.

We report generic and tuneable CAR in a superconductor sandwiched between two antiferromagnetic layers. We consider recent examples of two-dimensional magnets with hexagonal lattices, where gate voltages control the carrier type and density, and predict a robust signature of perfect CAR in the nonlocal differential conductance with one electron-doped and one hole-doped antiferromagnetic lead. The magnetic field-free and spin-degenerate CAR signal is electrically controlled and visible over a large voltage range, showing promise for solid-state quantum entanglement applications.

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## **Topological Hall effects due to Skyrmions in Antiferromagnets**

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It is well known that THE in ferromagnetic materials can be described by the Berry phase acquired by the electron wavefunction, when the electron spin follows adiabatically the local nontrivial magnetic texture (e.g. skyrmion texture) [1,2,3,4]. In this description, the influence of the magnetic texture is characterized by an emergent magnetic field, which leads to a spindependent force acting on the itinerant electrons. We have studied theoretically the topological Hall effect (THE) as well as the topological spin Hall effect (TSHE) due to Skyrmions in twodimensional antiferromagnets (AFMs) - both collinear and noncollinear. In collinear antiferromagnets, the THE was shown to disappear, while TSHE was found to be nonzero [4,5]. However, it was shown recently, that both TSHE and THE may occur in collinear antiferromagnets, when relaxation processes are spin-dependent [6]. Such a spin asymmetry in scattering processes may appear, e.g., due to magnetic impurities. However, a non-zero magnetization due to canting of the sublattice magnetic moments in uncompensated antiferromagnets lifts the spin degeneracy and splits the conduction (and also valence) band into two spin subbands. As a result, both TSHE and THE may exist in such AFMs - also in the absence of relaxation time asymmetry. Dispersion curves of the split conduction band resemble those for Rashba spin-orbit system. Depending on the Fermi level position, one can distinguish then two transport regimes: (i) when both spin subbands contribute to transport, and (ii) only one spin subband takes part in transport. Using the semi-classical Boltzmann approach, we have derived the diffusion equation for the spin accumulation in the presence of spin-flip scattering. The gradient of the emergent magnetic field acts then as a source for spin accumulation, which occurs within the area of a Skyrmion. As a result, we have found the corresponding TSHE as well as the THE, and analysed in detail their dependence on the total magnetization, spin-flip scattering, and Skyrmion size. Our results also indicate that changes in the Fermi level from the two-spin states to the single-spin state have an important effect on the behaviour of the topological Hall effects.

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## Magnons in the VX<sub>2</sub> (X=S, Se, Te) monolayer and bilayer TMD systems

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We have analyzed theoretically the spectrum of spin waves in two-dimensional monolayer and bilayer systems of VX<sub>2</sub> (X=S, Se, Te) transition-metal dichalcogenides (TMDs). The Vanadium atoms within individual atomic layers are coupled ferromagnetically. Additionally, in case of the bilayer system, the exchange coupling between V atoms located in different planes is either ferromagnetic or antiferromagnetic, depending on the type of dichalcogenide (X) atom [1]. We have analyzed the magnon spectra as a function of magnetic anisotropy, external magnetic field, and Dzyaloshinskii-Moriya interactions. The spin-wave dispersion relations have been derived analytically within the spin-wave theory, in terms of the Holstein-Primakoff transformation combined with the Bogolubov diagonalization scheme [2,3].

In the case of bilayers with antiferromagnetic interlayer coupling, the system undergoes a fieldinduced transition to the spin-flop phase, which evolves into the saturated ferromagnetic phase for sufficiently strong magnetic fields. The existence of different phases depends on the interlayer exchange parameters and anisotropy constants. We have shown how spin-wave spectra change at the phase transitions and how they evolve with increasing magnetic field. We have taken into account both, in-plane and out-of-plane magnetic anisotropy as well as in-plane DMI. The latter leads to nonreciprocal spin-wave propagation.

Transition of magnetization from in-plane to out-of-plane orientation in VSe<sub>2</sub>-NiSe<sub>2</sub> heterostructure [4] led to further discussion on the interplay between intralayer exchange interactions, and strong out-of-plane magnetocrystalline anisotropy, and on their influence on the spin wave-spectra. Due to the proximity effect, the discussion also includes the description of a specific behaviour of magnons in the presence of Dzyaloshinskii-Moriya interactions.

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# Magnetic properties of Vanadium-based Transition metal dichalcogenides

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Density Functional Theory (DFT) was employed to investigate the electronic and magnetic characteristics of monolayer and bilayer structures of Vanadium-based dichalcogenides VX<sub>2</sub> (X=S, Se, Te) in the hexagonal (H) phase. The monolayers display ferromagnetic ordering, which changes to antiferromagnetic (AFM) one when the number of layers increases - with the exception of VS2. To evaluate basic parameters of these materials, both GGA+U and GGA+SOC approaches were used in the DFT calculations. Magnetic anisotropy and exchange parameters were computed to estimate the Curie temperature and determine the spin wave energy using the relevant spin Heisenberg Hamiltonian. Additionally, the magnetic properties of a T-phase bilayer VS<sub>2</sub> under a mechanical bi-axial strain were explored. The achieved results provide insight into the electronic and magnetic complexities of Vanadium-based transition metal dichalcogenides, and also highlight their potential for applications in spintronic devices - e.g., in spin-valve systems [1-5].

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## Spin-orbit coupling driven phenomena in twisted graphene on transition metal dichalcogenides

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Twisted bilayer graphene and its extraordinary phase transitions observed at a magic twist angle initiated a new and promising research area called twistronics. Controlling twisting angle in case of layered structures, like van-der-Waals heterostructers, can lead to other interesting transport properties in which electric or spin signals can be tuned externally. Twisted structures containing graphene and semiconducting transition metal dichalcogenides (TMDCs) create opportunities to observe proximity induced spin-orbit coupling that varies with the twist angle leading to different response for spin-orbit coupling driven phenomena.

We will present a theoretical analysis of various effects that emerge due to spin-orbit coupling, like spin Hall effect [1] and current-induced spin polarization, in twisted graphene deposited on selected TMDCs such as MoS<sub>2</sub>, WS<sub>2</sub>, MoSe<sub>2</sub>, and WSe<sub>2</sub>, modelled by an effective Hamiltonian derived from symmetry analysis and DFT calculations (see e.q., [2-4]). We will discuss the angle dependence of these effects as well as behavior of Berry curvature that impacts the valley dependent transport properties. Our study and analytical formulas are applicable to various TMDCs materials.

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## Magnetism of CrX<sub>3</sub> hexagonal layers win the atomistic spin dynamics

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Chromium trihalides, CrX<sub>3</sub> (X=I, Cl, Br), are van der Waals materials with interesting topological and magnetic properties. The Cr atoms in individual monolayers of these compounds form a hexagonal lattice [1,2]. Since the interlayer exchange coupling in these materials is relatively weak, they serve as a playground for studying monolayers, bilayers with a variety of offsets, twisted layers, as well as for investigating external tuning of their properties with strain or electric fields [3]. The main focus of the talk is on the magnetic properties of CrI<sub>3</sub> in the monolayer as well as bilayer forms. An important issue is the influence of layer stacking on the Curie temperatures, hysteresis loops, spin textures, and magnon spectra in CrI<sub>3</sub> bilayers. More specifically, we consider two different stackings, i.e., the AA and Rhombohedral ones.

The magnetic properties have been studied within the atomistic spin dynamics (ASD) approach [4]. This approach is based on the classical spin models and Landau-Lifshitz Gilbert equations for individual spins. In our investigation, the spin models include the exchange couplings, Dzyaloshinskii-Moriya interaction, magnetic anisotropy, and local/external magnetic fields. To evaluate the Critical temperature we use the ASD methods to simulate temperature dependence of the magnetization, magnetic susceptibility, and specific heat. As for the hysteresis curves and the associated spin patterns, our main focus is on the search for parameters that are suitable for formation of specific spin patterns, like stripes and individual skyrmion textures. Finally, the ASD simulation methods are used to investigate magnon dispersion relations and their behaviour in specific points and along specific orientations of the first Brillouin zone.

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## Topological magnon gap engineering in 2D van der Waals CrI<sub>3</sub> ferromagnets

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The microscopic origin of the topological magnon band gap in CrI3 ferromagnets has been a subject of controversy for years since two main models with distinct characteristics, i.e., Dzyaloshinskii-Moriya (DM) and Kitaev, provided possible explanations with different outcome implications. Here we investigate the angular magnetic field dependence of the magnon gap of CrI<sub>3</sub> by elucidating what main contributions play a major role in its generation. We implement stochastic atomistic spin dynamics simulations to compare the impact of these two spin interactions on the magnon spectra. We observe three distinct magnetic field dependencies between these two gap-opening mechanisms. First, we demonstrate that the Kitaev-induced magnon gap is influenced by both the direction and amplitude of the applied magnetic field, while the DM-induced gap is solely affected by the magnetic field direction. Second, the position of the Dirac cones within the Kitaev-induced magnon gap shifts in response to changes in the magnetic field direction, whereas they remain unaffected by the magnetic field direction in the DM-induced gap scenario. Third, we find a direct-indirect magnon band-gap transition in the Kitaev model by varying the applied magnetic field direction. These differences may distinguish the origin of topological magnon gaps in  $CrI_3$  and other van der Waals magnetic layers. Our findings pave the way for exploration and engineering topological gaps in van der Waals materials.

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## Non-linear anomalous Hall effect in a 2DEG with different forms of Rashba spin-orbit interaction

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Recently, non-linear transport phenomena have been attracting much attention due to their application potential in spin-logic devices [1]. Moreover, the intrinsic type of the non-linear Hall effect (NLHE), related to the Berry curvature dipole, is sensitive to the symmetry breaking in the system. Therefore, NLHE turned out to be very useful for material characterization and also in strain sensors [2].

Here, we provide a theoretical description of the NLHE in a magnetized 2DEG with various forms of Rashba spin-orbit interaction. As the well-known k-linear form of Rashba coupling is applicable to semiconductor heterostructures, the interfaces and surfaces of perovskite oxides (e.g., LaAlO<sub>3</sub>/SrTiO<sub>3</sub>) and p-doped semiconductor heterostructures reveal k-cubed forms of Rashba spin-orbit interaction [3]. We demonstrate here, among others, that the NLHE in such systems can be tuned with an external in-plane magnetic field [4].

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## Bilinear magnetoresistance and planar Hall effect in topological insulators: interplay of scattering on spin-orbital impurities and nonequilibrium spin polarization

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Nonlinear transport phenomena, such as the bilinear magnetoresistance (BMR) and nonlinear planar Hall effect (NPHE), are currently of great interest. We propose a possible microscopic mechanism that gives rise to these phenomena in topological insulators (TIs) [1]. This mechanism is associated with scattering on impurities that inherently possess spin-orbit coupling. By employing the Green's functions formalism and diagrammatic method, we have successfully obtained analytical results for both the diagonal and off-diagonal conductivities, that allowed us to determine the nonlinear signals. These analytical findings, combined with numerical results, shed light on the potential of utilizing simple magnetotransport measurements to accurately determine the material constants, such as the Fermi wavevector and the spin-orbit coupling parameter.

It should be noted that BMR and NPHE in TIs may have two other important mechanisms that have been studied recently. The first one is related to the presence of nonzero second-order spin currents in systems with anisotropic Fermi contours [2]. The second one is based on the interplay of an effective spin-orbital field (related to the non-equilibrium spin polarization) and specific scattering due to inhomogeneity in the spin-momentum locking [3]. Interestingly, the latter mechanism can also manifest itself in systems with isotropic Fermi contours. To verify reliability of the proposed model, we compare our results with those obtained in other models.

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Acknowledegments: This work has been supported by the National Science Centre in Poland under the project Sonata-14 no. 2018/31/D/ST3/02351.

## January 31st

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Sessions 6-7

## Fermi level control in topological insulators

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#### M. Chrobak<sup>1,2</sup>, K. Nowak<sup>1,2</sup>, A. Naumov<sup>2</sup>, A. Trembułowicz<sup>2</sup>, T. Parashchuk<sup>3</sup>, B. Wiendlocha<sup>1</sup>, K. Wojciechowski<sup>3</sup>, and <u>M. Przybylski<sup>1,2</sup></u>

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Topological insulators (TIs) like single-crystalline  $Bi_2Se_3$  and  $Bi_2Te_3$  possess unique properties of metallic surface states, such as the Dirac-cone structure and an insulating/semiconducting volume, which pave the way for advanced technologies. However, the practical applications of TIs are still limited due to the insufficient control over the details of their electronic structure. In particular, defects arising from the growth conditions result in the Fermi level ( $E_F$ ) being located not in the gap but in the volume electronic bands [1], [2].

We show that neither control over the density of defects nor over the dopant concentration is sufficiently efficient to shift the  $E_F$  to the gap as small deviations from the stoichiometry. We report the results of a variety of experiments like Scanning Tunneling Microscopy (STM; helping to identify the existing defects and their density), Scanning Tunneling Spectroscopy (STS; helping to identify the electronic structure at surfaces), Scanning Thermoelectric Microprobe (SThM; to verify the carrier concentration and its distribution) and Shubnikov de Haas (SdH) oscillations at very low temperatures (to identify the Berry phases and oscillation frequencies corresponding to the volume and surface electronic states).

Our experimental results are verified with Density Functional Theory (DFT) calculations of the volume electronic structure. The calculations were performed based on the densities of various structural defects (derived from the STM experiment) and verified with the carrier concentration (derived from the Hall resistivity) and compared to the SThM maps taken for the selected Bi<sub>2-x</sub>Te<sub>3+x</sub> samples. The unimodal Gaussian function was used to fit the Seebeck coefficient histogram, while the standard deviation was chosen and is discussed as a parameter that represents the uniformity of the Seebeck coefficient (i.e., of the carrier concentration). The frequencies of the measured SdH oscillations were derived and attributed to the conduction and valence volume bands and to the topologically non-trivial surface states, and then discussed as a function of the carrier concentration [3].

Finally, we have tried to control the position of the  $E_F$  by voltage applied to flakes a few nanometers thick, which is challenging from an experimental point of view. We report on the results of the anomalous Hall effect and on the resistivity measured along the applied voltage for  $Bi_2Te_3$  flakes doped with Mn. Since the contacts were made of aluminum, locally induced superconducting (SC) properties were obtained and are discussed as a function of the external magnetic field and of the current flowing through such SC/TI junctions at low temperatures at which Al is superconducting.

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## Connection between the semiconductor-superconductor transition and the spin-polarized superconducting phase in the honeycomb lattice

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The realization of the honeycomb lattice in graphene draws a lot of attention of the scientific community. The extraordinary properties of the honeycomb lattice are mainly associated with massless Dirac fermions, which are located in the corners of the Brillouin zone. As a consequence, fermions in this lattice manifest a semiconducting behavior below some critical value of the onsite attraction, Uc. However, above Uc, the superconducting phase can occur.

This lattice exhibits also topological properties manifested by the existence of zero-energy edge states or in the quantum Hall effect, associated to the finite Berry curvature in these systems.

The electronic properties of the honeycomb lattices has opened new avenues of research in which applications play a very important role, i.e., spintronics or valleytronics.

Here, we discuss an interplay between the semiconductor – superconductor transition and the possibility of realization of the spin-polarized superconductivity (the so-called Sarma phase) [1,2].

We show that the critical interaction can be tuned by the next-nearest-neighbor (NNN) hopping in the absence of the magnetic field. Moreover, a critical value of the NNN hopping exists, defining a range of parameters for which the semiconducting phase can emerge.

In the weak coupling limit case, this quantum phase transition occurs for the absolute value of the NNN hopping equal to one third of the hopping between the nearest neighbors.

Similarly, in the presence of the magnetic field, the Sarma phase can appear, but only in a range of parameters for which initially the semiconducting state is observed.

Both of these aspects are attributed to the Lifshitz transition, which is induced by the NNN hopping as well as the external magnetic field.

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## Topological phase transition in 1D quantum spin system

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We will present a topological phase transition in the ground state  $\Psi_0$  of spin- $\frac{1}{2}$  Heisenberg antiferromagnet in a chain with nearest and next nearest neighbor  $\lambda$  interactions.

Firstly, it will be shown how to define winding numbers W (topological charges) in a onedimensional system in the basis of resonating valence bond states.

Secondly, it will demonstrated that the finite-size scaling of

- i) topological charge,  $\eta_T(\lambda) = \langle \Psi_0(\lambda) | W | \Psi_0(\lambda) \rangle$ ,
- ii) topological fidelity susceptibility,  $\chi_t(\lambda) = \frac{1}{L} \langle \partial_\lambda \Psi_0(\lambda) | W | \partial_\lambda \Psi_0(\lambda) \rangle$ ,
- iii) topological connection,  $\beta_t(\lambda) = \frac{1}{L} \langle \Psi_0(\lambda) | W | \partial_\lambda \Psi_0(\lambda) \rangle$

calculated dor finite systems of *L* spins leads to the accurate value of critical coupling  $\lambda_c = 0.2412 \pm 0.0007$  and to the value of subleading critical exponent  $\nu = 2.000 \pm 0.001$ .

This approach should be helpful when examining the topological phase transitions in all systems described not only in the resonating valence bond basis but also in the equivalent Projected Entangled Pair States.

### **Compact localised states in magnonics**

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In bipartite lattices, the sites from sublattice A have the nearest neighbours (NN) in sublattice B only. Therefore, the mods occupying one sublattice are not able to propagate (in tight-binding models with NN hopping) and the dispersion relation can be described as flat bands with zero group velocity. Such modes, localized without defects in a perfectly periodic and infinitely extended system, are called compact localized states (CLS) [1]. The well-known type of bipartite lattice is a Lieb lattice [2]. The CLS were already observed in photonic crystals based on Lieb lattices [3] but the studies on CLS in the magnonic system still need to be performed. We proposed a perpendicularly magnetized Ga-doped YIG layer as a base for a magnonic Lieb lattice where the lattice sites are mimicked by cylindrical inclusion made of YIG (without Ga-doping). We tailored the structure to observe the oscillatory and evanescent spin waves in inclusions and matrix, respectively. We calculated the dispersion relations exhibiting Dirac cones, almost touching each other at the M-point (with a very narrow gap ~15 MHz), intersected by a relatively flat band of magnonic CLS. Then, we supplemented our studies by considering the extended magnonic Lieb lattices, characterized by a larger number of weakly dispersive bands specific for CLS. The computations were performed by finite element method, using COMSOL Multiphysics.

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## Magnetization dynamics in two-dimensional ferromagnets

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#### Witold Skowroński<sup>1,2</sup>, Mayank Sharma<sup>2</sup>, Marco Gobbi<sup>2,3</sup>, Felix Casanova<sup>2,4</sup>, Luis Hueso<sup>2,4</sup>

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Two-dimensional (2D) materials enable unique multilayer system stacking, high interface-tobulk ratio and unconventional types of symmetry breaking mechanisms. It has been presented, that by using a combination of 2D layer with high spin-orbit coupling (WTe2) and ferromagnet (Py), the symmetry of spin-orbit torque can be controlled [1]. In addition to transition-metal dichalcogenides ferromagnetic materials can also be synthesised in a form of van der Waals crystals, which are characterized by very high perpendicular magnetic anisotropy and anomalous Hall effect (AHE) [2]. However, determination of other properties of the magnetic materials, such as magnetization damping or saturation magnetization remains challenging, as typically, 2D magnets are fabricated in form of irregular and mm-size flakes.

In the present work, I will summarize the investigation of 2D-materials hybrids using static and dynamical measurement methods. I will show AHE and spin-Hall effect in FeGeTe/Pt bilayer and point out the crucial role of the interface between two layers. Next, I will move to the magnetization dynamics measurement of the CrGeTe/Pt using ferromagnetic resonance spectroscopy and spin-diode effect. An update of the spin-pumping effect in CeGeT exhibiting very low damping will be presented [3]. The talk will be concluded by current challenges and prospects of the magnetization dynamics in van der Waals ferromagnets.

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## A First-Principles Study of Magnetic Properties and Structural Phase Transitions in Ultra-Thin Fe Films

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Iron-based layered systems are of great interest due to their ability to adjust magnetic anisotropy energy (MAE) and other material parameters. The crystallographic structure of Fe, its thickness, and the presence of other layers above and below the Fe layer can significantly affect magnetic parameters, such as the MAE. This topic is important from an application point of view.

We describe how changes in the Fe layer thickness affect its structural and magnetic properties. The density functional theory (DFT) implemented in the full-potential local-orbital (FPLO) code [1] was used to calculate the properties of these structures. The layers' structures underwent optimization of the interlayer spacings' geometry. Equilibrium structures were then recalculated using a fully relativistic approach for two orthogonal magnetization directions (in-plane and perpendicular to the plane of the layer).

The impact of the number of Fe monolayers on the lattice parameters and magnetic properties of the system is analyzed. It is demonstrated that the MAE can have different signs and values depending on the number of Fe monolayers. The behavior of the density of states for these systems is also studied. Additionally, the distribution of spin magnetic moment and electric charge within the thin films is examined.

A structural phase transition is observed in free Fe layer calculations. This phase transition occurs in Fe layers with different surfaces, such as bcc (001), fcc (111), or bcc (111), and at varying thicknesses of Fe layers [2].

Additionally, we conducted a theoretical study on the magnetic anisotropy of ultrathin FeCo films, which are only 9 atomic monolayers thick. The films were doped with B, C, and N, which were located in the octahedral interstitial position at the center of the layer [3]. In contrast to bulk systems, our findings suggest that doping FeCo with B, C, and N atoms in the octahedral position in 9-atomic-monolayer thick FeCo films can significantly reduce the MAE, even changing its sign to negative in the case of B-doped FeCo thin films. These results have important implications for further research on magnetic thin films for spintronic applications.

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## Impact of ion bombardment on ferrimagnetic Tb/Co multilayers using different ion species

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#### D. Kiphart<sup>1</sup>, M. Krupiński<sup>2</sup>, M. Mitura-Nowak<sup>2</sup>, M. Kowacz<sup>1</sup>, M. Schmidt<sup>1</sup>, F. Stobiecki<sup>1</sup>, P. Kuświk<sup>1</sup>

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Interest in ferrimagnetic rare earth (e.g., Tb)-transition metal (e.g., Co) thin films has been rekindled for applications in all-optical switching of magnetization and spintronics [1,2]. We have previously shown that 10 keV He+ ion bombardment (IB) through a photoresist mask can be used to locally modify the magnetic properties of Tb/Co multilayers [2,3]. It was shown that this is primarily due to preferential oxidation of Tb. However, other mechanisms have been also suggested, such as the reduction of short-range chemical order, interlayer mixing and segregation of Tb [1-6]. Therefore, there are outstanding questions about the mechanism by which this selective deactivation of Tb takes place.

In this contribution, we present the results from IB using different ion species with similar energies (i.e., 10 keV He+, 15 keV O+ and 30 keV Ga+). The choice of ion species and fluence enables the effective composition of the films to be tailored by Tb deactivation and therefore changing the magnetic properties of the Tb/Co multilayer after IB (e.g., sublattice domination, coercivity and effective magnetization). We show that this change in effective composition of the show that this change in effective composition of the experimental data with IB Monte-Carlo simulations using the TRIDYN code [7] indicates that this is primarily due to microstructural damage which allows creation of easy diffusion paths for oxygen penetration after IB.

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2D Quantum Materials for Spintronics, 2DQMS 29<sup>th</sup> – 31<sup>st</sup> January 2024 Poznań, Poland CONCERNMENT (CARACTER CONCERNMENT)

## Poster session

No. Marrison

## Neural network quantum states analysis of the Shastry-Sutherland model

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#### M. Mezera<sup>1,2</sup>, J. Menšíková<sup>3,4</sup>, <u>P. Baláž</u><sup>3</sup>, M. Žonda<sup>1</sup>

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We present a comprehensive study on the application of neural network quantum states (NQS) [1] for analyzing the ground state properties of the quantum Heisenberg model on a Shastry-Sutherland lattice [2] (see Figure). By employing the variational Monte Carlo method, the study demonstrates that even relatively simple NQSs can effectively approximate the ground state of the model across various phases and regimes. Initial investigations involved comparing multiple NQS types on smaller lattice systems, benchmarking their variational energies against results obtained from exact diagonalization.



The research finds that, considering factors such as precision, generality, and computational efficiency, a shallow restricted Boltzmann machine (RBM) NQS emerges as a favorable choice for larger system applications. This particular NQS effectively describes the main phases of the model in the absence of a magnetic field; dimer state (DS), plaquette state (PS), antiferromagnetic state (AF). Additionally, the study reveals that an NQS based on a restricted Boltzmann machine can accurately capture the formation of magnetization plateaus in the model as the magnetic field strength increases. These findings highlight the potential of NQS in providing insightful analyses in complex quantum systems [3].

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## 

## Localized states at the Rashba spin-orbit and magnetic domain walls in graphene: topological properties

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It is well known that when both Rashba spin-orbit coupling (SOC) and magnetizations are nonzero and uniform in graphene, then a gap in electronic spectrum of graphene is open at the Dirac points [1]. Here, we consider first the situation, when either magnetization or Rashba SOC form a domain wall [2]. Solving the relevant Schrodinger equation, we find electronic states localized at the Rashba or magnetic domain wall, that emerge in the gap. However, the states localized at the magnetic and Rashba domain walls have different topological properties.

Then, we analyse the coexistence of both domain walls at the same position and analyse the corresponding localized states. We show, that when a magnetic domain wall is present, then the localized states describe the Quantum Anomalous Hall Phase (QAHP), independently if the Rashba coupling forms a domain wall or only a step. The localized states cross then the gap and connect the valence and conduction bands. In turn, when the magnetization does not form a domain wall, then independently of whether the Rashba SOC forms a domain wall or not, the localized states do not display topological properties [3]. Apart from equilibrium currents relevant for QAHP, we also analyse nonequilibrium charge and spin currents flowing along the domain wall due to voltage or temperature gradient.

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2D Quantum Materials for Spintronics, 2DQMS 29<sup>th</sup> – 31<sup>st</sup> January 2024

## Phase-space entropic indicators of the topological phase transitions in silicene

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When subjected to an external field, 2D materials described by the Kane-Mele Hamiltonian may undergo a topological phase transition. Silicene, recognized as a topological insulator (TI), exhibits a shift to a band insulator (BI) when influenced by the interplay of spin-orbit coupling and an external field. Recent studies reveal that information metrics such as Fisher information, complexity measure, or Rényi entropy can serve as indicators for such topological phase transitions (TPT) [1].

Conversely, the phase-space formulation of quantum mechanics, utilizing the Wigner distribution function (WDF), is widely applied and gaining popularity in condensed matter physics [2], especially in the context of two-dimensional materials interacting with magnetic and electric fields [3]. In our research, we have computed an analytical expression for the WDF of silicene interacting with a perpendicular magnetic field. This outcome has enabled the utilization quantum entropic measure based on the WDF to identify TPTs in the system and characterize the topological state of matter with Wigner-Rényi's phase-space entropy.

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

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Topological insulators are quantum materials that are currently of great interest from both fundamental and application points of view. This interest is a consequence of their unique electronic and transport properties, like for instance dissipationless transport which may play an important role in future applications in spintronics, nanoelectronics, and information technology [1]. Moreover, topological insulators are excellent candidates for observing some exotic quantum phenomena, e.g., the surface topological states and quantum anomalous Hall effect.

In our work, we consider a heterostructure consisting of a thin layer of topological insulator, sandwiched between two ferromagnetic layers. This breaks the time-reversal symmetry [2] and allows to observe the quantum anomalous Hall effect. Each of the magnetic layers is characterized by the direction of magnetization along the axis normal to the layers. Magnetization direction can be changed in two ways — by applying an external magnetic field or by changing the hybridization parameter that is related to the thickness of the topological insulator. Using the Green function formalism and Kubo formula, we calculate the topological and transport properties of such systems, e.g., anomalous Hall conductivity, topological phase transition, and current-induced spin polarization.

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### **Dynamical Hall responses of disordered superconductors**

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We extend the Mattis-Bardeen theory [1] for the dynamical response of superconductors to include different types of Hall responses. This is possible thanks to a recent modification of the quasiclassical Usadel equation [2,3], which allows for analyzing Hall effects in disordered superconductors and including the precise frequency dependence of such effects. Our results form a basis for analyzing dynamical experiments especially on novel thin-film superconductors, where ordinary Hall and spin Hall effects can both show up.

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# Bilinear magnetoresistance and planer Hall effect in topological insulators: contribution from scattering on magnetic impurities

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Bilinear magnetoresistance and bilinear planar Hall effect [1-3] are two nonlinear transport phenomena that scale linearly with the electric and magnetic fields, and appear in non-magnetic systems with strong spin-orbit coupling, such as topological insulators (TIs). Using the semiclassical Boltzmann theory and generalized relaxation time approximation, we have considered in detailed both the bilinear phenomena. The description has been based on an effective model describing surface states of three-dimensional topological insulators. Assuming that magnetic moments of the impurities in the system follow the external magnetic field orientation [4], we have shown that the bilinear magnetoresistance and the nonlinear Hall conductivity become remarkably modified by scattering on magnetic impurities. The interplay of electron scattering on scalar and magnetic impurities results, among others, in additional periods in the variation of the corresponding currents with the magnetic field orientation.

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# Bilinear magnetoresistance in a 2DEG with isotropic cubic Rashba spin-orbit interaction

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The bilinear magnetoresistance (BMR) scales linearly with both the electric and magnetic fields applied to the system and is of potential application in spin-logic devices due to the corresponding unidirectional response [1]. In systems featuring strong Rashba-type spin-orbit interaction, BMR originates from effective spin-orbit field, that is related to non-equilibrium spin polarization [2].

In our study, we employ Green's function formalism to derive the analytical formula for BMR in a 2DEG with an isotropic cubic form of Rashba spin-orbit interaction and an external in-plane magnetic field [3]. The cubic form of Rashba coupling is suitable for modeling the surfaces or interfaces of perovskite oxides as well as p-doped semiconductor heterostructures [4]. Our findings reveal that BMR is characterized by  $2\pi$ -periodic oscillations with an in-plane magnetic field angle, and it can be tuned by adjusting both the strength of the Rashba spin-orbit interaction and the magnitude and direction of the external magnetic field. Moreover, this effect is observable even in weak magnetic fields [3].

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## Bilinear magnetoresistance and planar Hall effect in topological insulators: interplay of scattering on spin-orbital impurities and nonequilibrium spin polarization

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Nonlinear transport phenomena, such as the bilinear magnetoresistance (BMR) and nonlinear planar Hall effect (NPHE), are currently of great interest. We propose a possible microscopic mechanism that gives rise to these phenomena in topological insulators (TIs) [1]. This mechanism is associated with scattering on impurities that inherently possess spin-orbit coupling. By employing the Green's functions formalism and diagrammatic method, we have successfully obtained analytical results for both the diagonal and off-diagonal conductivities, that allowed us to determine the nonlinear signals. These analytical findings, combined with numerical results, shed light on the potential of utilizing simple magnetotransport measurements to accurately determine the material constants, such as the Fermi wavevector and the spin-orbit coupling parameter.

It should be noted that BMR and NPHE in TIs may have two other important mechanisms that have been studied recently. The first one is related to the presence of nonzero second-order spin currents in systems with anisotropic Fermi contours [2]. The second one is based on the interplay of an effective spin-orbital field (related to the non-equilibrium spin polarization) and specific scattering due to inhomogeneity in the spin-momentum locking [3]. Interestingly, the latter mechanism can also manifest itself in systems with isotropic Fermi contours. To verify reliability of the proposed model, we compare our results with those obtained in other models.

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## Intrinsic transport response in graphene-based EX-SO-TIC van-der-Waals heterostructures

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Two-dimensional van-der-Waals materials focus enormous attention due to a variety of electronic and magnetic properties, that might be controlled by external fields. A special group of van-der-Waals materials are so-called ex-so-tic structures, where one can turn the time-reversal symmetry on and off on demand by electric gating. This leads to the swap between an exchange (ex) and spin-orbit (so) coupling. An example of such an ex-so-tic structure is a bilayer graphene (GG) sandwiched by a 2D ferromagnet  $Cr_2Ge_2Te_6$  (CGT) on one side and a monolayer of transition metal dichalcogenides (e.g., WS<sub>2</sub>) on the other side. Swapping between the exchange and spin-orbit coupling in CGT/GG/WS<sub>2</sub> is possible due to the interplay of gate dependent layer polarization in the graphene bilayer, and short-range spin-orbit and exchange proximity effects affecting only the monolayer of graphene in direct contact with the adjacent materials.

Within an effective Hamiltonian derived from symmetry considerations and DFT study [1], we derived electronic and topological properties of CGT/GG/WS<sub>2</sub>. We present, among others, the behavior of Berry curvature as a function of characteristic parameters defining the Hamiltonian and discuss possible topological phase transitions for the ex-so-tic structure. Furthermore, we present detailed characteristics of the intrinsic anomalous, spin and valley Hall effects [2] that may appear in specific phases.

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## Magnon dispersion from atomistic spin dynamics

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The atomistic spin dynamic (ASD) approach [1] may be considered as a bridge between micromagnetism and the abinito methods. While the effective parameters originate from the density functional analysis, the numerical methods are applied to the classical models, similarly as in the micromagnetism. Taking into account full geometry of the system, allows one to investigate different physical properties in various layer stackings. The method works fast in small systems, and is a useful tool for finding and illustrating spin textures in the system, ground states, and the dynamics due to a magnetic perturbation. The latter is useful in calculation of the magnon dispersions directly from the spin dynamic. Similar results can be achieved from calculating the spin correlations and dynamical structure factor.

The main focus of the poster is to provide a technical inside into the magnon dispersion calculations. The discussion includes different excitation possibilities and damping of the dynamics. The described method is applicable to distorted materials, defects, and impurities. It can be also used to systems of any geometry. While many established theoretical methods are suitable for the linearized system, the direct method allows to study non-linear effects without further simplification, as well as the dispersions in the presence of pseudo-stable texture. This method is also useful when analyzing the magnon dispersion with switching capabilities.

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## First-principle Analysis of Electronic and Transport Properties in Finite Nanoribbons and Nanodiscs of selected 2D Materials

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We used the density functional theory (DFT) to explore the complex electronic structures and transport behaviour of various nanoribbons and nanodiscs from specific two-dimensional materials, like graphene, silicene, and hexagonal boron nitride (h-BN). The main emphasis was on the identification and examination of zero-energy states (ZESs), which play a crucial role in understanding chirality-related topological properties. Additionally, we also investigated transport properties of these nanostructures. Our results uncover a diverse array of ZESs in these nanostructured 2D materials, where their presence and features are strongly influenced by such factors like edge geometry, material type, and dimensionality. Furthermore, we explored the influence of ZESs on transport properties, illustrating their potential to enhance charge carrier mobility and conductivity. This thorough exploration significantly contributes to advancing our knowledge of the fundamental electronic properties and transport behaviour of 2D material-based nanostructures, offering insights for the development of innovative nanoelectronic devices and applications [1-6].

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