MA 29: Spin-Dependent Phenomena in 2 D

Time: Wednesday 15:00–19:00 Location: EB 202

MA 29.1 Wed 15:00 EB 202

Is NiPS3 a good candidate to see the Berezinskii-Kosterlitz-Thouless transition? — •Yangjun Lee[1,2,3], Tae Yun Kim[2], and Cheol-Hwan Park[1,2,3] — [1]Department of Physics and Astronomy, Seoul National University, Seoul 08826, Korea — [2]Center for Correlated Electron Systems, Institute for Basic Science, Seoul 08826, Korea — [3]Center for Theoretical Physics, Seoul National University, Seoul 08826, Korea

Magnetism in two-dimensional (2D) systems has been the subject of extensive study due to their distinct properties, which set them apart from three-dimensional (3D) systems. The Mermin-Wagner theorem asserts that continuous symmetry cannot be spontaneously broken in a 2D system in finite temperature. Nonetheless, the XY model, which exhibits continuous symmetry, demonstrates a phase transition at a nonzero temperature known as the Berezinskii-Kosterlitz-Thouless (BKT) transition. Recently, few-layer transition metal phosphorus trichalcogenides have garnered interest for their potential to exhibit intriguing 2D magnetic properties. Specifically, NiPS3 is regarded as an exemplar of XY model magnetism [1]. In this presentation, we will examine whether NiPS3 could be considered a promising candidate for observing the BKT transition [2, 3]. [1] Kim, K., Lim, S.Y., Lee, JU. et al. Nat. Commun. 10, 345 (2019). [2] T.Y. Kim and C.-H Park. Nano Lett. 21, 10114 (2021). [3] Y. Lee, T. Y. Kim, and C.-H. Park, unpublished.

MA 29.2 Wed 15:15 EB 202

An Effective Magnetic Model for FePS3 — •Minsu Ghim, Tae Yun Kim, and Cheol-Hwan Park — Department of Physics and Astronomy, Seoul National University, Seoul, Korea

Two-dimensional (2D) magnetism has drawn attention due to its properties distinct from those in three-dimensional magnetic systems. One of the most notable features is the Mermin-Wagner theorem, which states that with isotropic Heisenberg interactions, long-range magnetic order cannot exist at finite temperatures in a 2D system. Despite the Mermin-Wagner theorem, long-range magnetic order can still arise due to magnetic anisotropy. To understand 2D magnetism, extensive studies have been focused on establishing a model Hamiltonian for various materials. It is essential to develop an accurate magnetic energy model not only to characterize the ground state but also to explain phase transitions or low-energy excitations such as magnons. In this study, we focus on the magnetism of single-layer FePS3. We calculate the total energies and magnetic moments of various spin configurations. We conduct a quantitative analysis of the exchange interactions and discuss how FePS3 achieves its known ground state, the zigzag-type antiferromagnetism. [1, 2]

[1] T. Y. Kim, and C.-H. Park, Magnetic Anisotropy and Magnetic ordering of Transition-Metal Phosphorus Trisulfides, Nano Lett. 2021, 21, 23, 10114-10121 [2] M. Ghim, T. Y. Kim, C.-H. Park, unpublished

MA 29.3 Wed 15:30 EB 202

Topological magnon gap engineering in layered van der Waals ferromagnet CrI3 — •Verena Brehm[1], Pawel Sobieszczyk[2], Jostein Kløgetvedt[1], Richard F. L. Evans[3], Elton J. G. Santos[4], and Alireza Qaiumzadeh[1] — [1]NTNU Trondhem, Norway — [2]Polish Academy of Sciences Krakow, Poland — [3]University of York, United Kingdom — [4]University of Edinburgh, Untied Kingdom

We investigate the angular magnetic field dependence of the topological magnon gap at the K-points of the ferromagnetic van der Waals insulator CrI3, by examining two gap-opening terms: the Dzyaloshinski-Moriya and Kitaev interaction. Using stochastic atomistic spin dynamics simulations and linear spin wave theory, we compare the impact of the two spin interactions on the magnon spectra in a single layer. We observe three distinct magnetic field dependencies between these two topological magnon gap opening mechanisms that may distinguish the origin of the topological magnon gap. 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, our findings reveal that the position of the Dirac cones within the Kitaev-induced magnon gap shifts dependent on the magnetic field direction, whereas they remain unaffected 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.

MA 29.4 Wed 15:45 EB 202

Electrical engineering of topological magnetism in two-dimensional heterobilayers — •Nihad Abuawwad[1,2], Manuel dos Santos Dias[3], and Samir Lounis[1,2] — [1]Peter Grünberg Institute (PGI), FZJ, 52425 Jülich, Germany — [2]Faculty of Physics, University of Duisburg-Essen, 47053 Duisburg, Germany — [3]Scientific Computing Department, STFC Daresbury Laboratory, Warrington WA4 4AD, United Kingdom

The emergence of topological magnetism in 2D van der Waals (vdW) materials has made 2D heterostructures vital for advanced information technology devices. Here, we show from first-principles calculations in combination with atomistic spin models that an external electric field modifies the vdW gap between $CrTe_2$ and (Rh, Ti)Te_2 layers and alters the underlying magnetic interactions. We demonstrate the all-electric switching of the topological nature of individual topological magnetic objects emerging in 2D vdW heterobilayers. The electric field enables switching between ferromagnetic skyrmions and meron pairs in the $CrTe_2/RhTe_2$ heterobilayer while it enhances the stability of frustrated antiferromagnetic merons in the $CrTe_2/TiTe_2$ heterobilayer. This discovery opens possibilities for energy-efficient information storage and transmission in spintronics [1,2,3].

–Work funded by the Palestinian-German Science Bridge (BMBF–01DH16027), and SPP 2244 (project LO 1659/7-1).

[1] arXiv:2311.01294, (2023). [2] Phys.Rev.B 108,094409 (2023). [3] J. Phys.: Condens. Matter 34 454001 (2022).

MA 29.5 Wed 16:00 EB 202

Magnetic Properties of Non-van der Waals 2D Materials — Tom Barnowsky[1,2], Mahdi Ghorbani-Asl[1], Thomas Heine[1,2], Stefano Curtarolo[3], Arkady V. Krasheninnikov[1,4], and •Rico Friedrich[1,2,3] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Dresden — [2]TU Dresden — [3]Duke University, Durham, USA — [4]Aalto University, Aalto, Finland

While 2D materials are traditionally derived from bulk layered crystals bonded by weak van der Waals (vdW) forces, the recent surprising experimental realization of non-vdW 2D compounds obtained from non-layered transition metal oxides [1] foreshadows a new direction in 2D systems research.

As outlined by our recent data-driven investigations [2, 3], these materials exhibit unique magnetic properties owing to the magnetic cations at the surface of the sheets. Despite of several ferromagnetic candidates, even for the antiferromagnetic representatives, the surface spin polarizations are diverse ranging from moderate to large values modulated in addition by ferromagnetic and antiferromagnetic in-plane coupling. At the same time, chemical tuning by surface passivation provides a valuable handle to further control the magnetic properties of these novel 2D compounds [4] thus rendering them an attractive platform for fundamental and applied nanoscience.

[1] A. Puthirath Balan *et al.*, Nat. Nanotechnol. **13**, 602 (2018).
[2] R. Friedrich *et al.*, Nano Lett. **22**, 989 (2022).
[3] T. Barnowsky *et al.*, Adv. Electron. Mater. **9**, 2201112 (2023).
[4] T. Barnowsky *et al.*, submitted, arXiv:2310.07329 (2023).

MA 29.6 Wed 16:15 EB 202

Emergence of the Unconventional Magnetic Order in Twisted Double Bilayer CrI3 (Part 2) — •Ruoming Peng[1], King Cho Wong[1], Eric Anderson[2], Sarah Jenkins[3], Xiaodong Xu[2], Elton Santos[3], and Joerg Wrachtrup[1] — [1]3. Physikalisches Institut, University of Stuttgart, 70569 Stuttgart, Germany — [2]Department of Physics, University of Washington, Seattle, WA 98195, USA. — [3]Institute for Condensed Matter Physics and Complex Systems, School of Physics and Astronomy, The University of Edinburgh, Edinburgh, EH9 3FD, UK

The moiré superlattice in magnetic two-dimensional (2D) materials has revealed intriguing correlated and topological states. In the second part, we employ the scanning NV probe technique to investigate the antiferromagnetic domain of twisted double bilayer CrI3. Our study has shown that the magnetic competition in the moiré superlattice can contribute to the spontaneous periodic magnetic order in the twisted antiferromagnets. Notably, our observations include periodic antiferromagnetic texture with a period significantly larger than the moiré period and the emergence of the *skyrmion-like* lattices after a field cooldown process.

MA 29.7 Wed 16:30 EB 202

Emergence of the Unconventional Magnetic Order in Twisted Double Bilayer CrI3 (Part 1) — •King Cho Wong[1], Ruoming Peng[1], Joerg Wrachtrup[1], Eric Anderson[2], Xiaodong Xu[2], Elton Santo[3], and Sarah Jenkins[3] — [1]University of Stuttgart, Stuttgart, Germany — [2]University of Washington, USA — [3]University of Edinburgh, The United Kingdom

The twisted engineering of magnetic two-dimensional (2D) materials provides a controlled and versatile platform for exploring exotic correlated and topological states. Here, we employ the scanning NV probe technique to investigate the magnetic properties of twisted double bilayer CrI3. Our study has unveiled an unconventional ferromagnetic and antiferromagnetic behavior within the realm of twisted antiferromagnets. The manifestation of this magnetic order is underpinned by moiré-induced magnetic competition. Notably, our observations include a substantial domain wall width of approximately 100 nm and a consistent magnetization of 30 *b/nm^2 within small twisted-angle devices.

MA 29.8 Wed 16:45 EB 202

An all Phosphorene Lattice Nanometric Spin Valve — •Soumya Jyoti Ray — Indian Institute of Technology Patna

Phosphorene is a unique semiconducting two-dimensional platform for enabling spintronic devices integrated with phosphorene nanoelectronics. Here, we have designed an all phosphorene lattice lateral spin valve device, conceived via patterned magnetic substituted atoms of 3d-block elements at both ends of a phosphorene nanoribbon acting as ferromagnetic electrodes in the spin valve. Through First-principles based calculations, we have extensively studied the spin-dependent transport characteristics of the new spin valve structures. Systematic exploration of the magnetoresistance (MR) of the spin valve for various substitutional atoms and bias voltage resulted in a phase diagram offering a colossal MR for V and Cr-substitutional atoms. Such MR can be directly attributed to their specific electronic structure, which can be further tuned by a gate voltage, for electric field controlled spin valves. The spin-dependent transport characteristics here reveal new characteristics such as negative conductance oscillation and switching of the sign of MR due to change in the majority spin carrier type. Our study creates possibilities for design of nanometric spin valves, which could enable the integration of memory and logic for all phosphorene 2D processors.

15 min. break

MA 29.9 Wed 17:15 EB 202

Ferromagnetic Chromium Telluride Thin Films — Anna Tschesche, Pia Henning, and •Jasnamol Palakkal — Advanced Epitaxy, Institute of Materials Physics, Georg-August-University of Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

Chromium-based chalcogenides belong to the few 2D materials known for their intrinsic ferromagnetism [1]. Chromium telluride thin films (i.e. Cr_2Te_3, CrTe, $CrTe_2$) come under this exceptional class having ferromagnetic ground states with different transition temperatures (T_C) and perpendicular magnetic anisotropy (PMA) [2-4].

Being relevant properties for applications such as magnetic random access memory (MRAM) devices, our aim is to find the Cr_xTe_y 2D material with the highest T_C and PMA. We successfully fabricated (0001)-oriented thin films of hexagonal Cr_xTe_y on Al_2O_3 (0001) substrates using our hybrid pulsed laser deposition (PLD) setup, that allows us to vary the Te-content via the temperature of a molecular beam source. All films show strong PMA at 5 K, with an easy axis of magnetization along out of plane direction and the T_C ranges from 155 K to 297 K. Further experiments were conducted and detailed results of the Cr_xTe_y-series will be presented.

[1] S. Yu et al., Science and Technology of Advanced Materials, 23 (2022) 140-160.

[2] Y. Wen et al., Nano Lett., 20 (2020) 3130-3139.

[3] X. Zhang et al., Nature Communications, 12 (2021) 2492.

[4] H. Zheng et al., Appl. Phys. Lett., 122 (2023) 023103.

MA 29.10 Wed 17:30 EB 202

Half-metallic transport and spin-polarized tunneling through the 2D ferromagnet Fe_4GeTe_2 — •Anita Halder[1,2], Declan Nell[1], Antik Sihi[1], Stefano Sanvito[1], and Andrea Droghetti[1,3] — [1]Trinity College Dublin, Dublin, Ireland — [2]SRM University-AP, Amravati, India — [3]CNR-SPIN, at G. d'Annunzio University, Chieti, Italy

The discovery of ferromagnetic 2D van der Waals (vdW) materials, Fe_nGeTe_2 (FGT) (n=3-5), has attracted attention for spintronics applications due to their high Curie temperature. We theoretically study the spin-dependent transport properties of Fe_4GeTe_2 (FGT4) using density functional theory and Non-equilibrium Green's Functions. We show that the conductance perpendicular to the 2D vdW layer is half-metallic, i.e. entirely spin-polarized (SP). This high SP remains robust transitioning from bulk to a single layer. Additionally, a large SP current is observed when the system is driven out of equilibrium up to a significant bias. This spin-dependent transport is largely unaffected in the presence of spin-orbit coupling and electron-electron correlation effects. Leveraging the spin-filtering capability of monolayer FGT4 presents an opportunity for designing a magnetic tunnel junction (MTJ) using 2D vdW materials, offering high tunnel magnetoresistance (TMR). An MTJ device exploiting the vdW gap as an insulating barrier between two FGT4 layers achieves a TMR of almost 500%. These findings may inspire further theoretical and experimental studies for designing more realistic spintronic devices, replacing conventional FM with 2D vdW materials.

MA 29.11 Wed 17:45 EB 202

Understanding of Co and Ni doping in 2D Fe_5GeTe_2 magnets via first principles theory — •Biplab Sanyal[1], Soheil Ershadrad[1], Sukanya Ghosh[1,2], and Masoumeh Davoudiniya[1] — [1]Department of Physics & Astronomy, Uppsala University, Box.516, 75120 Uppsala, Sweden — [2]VIT Bhopal, India

In recent times, the family of 2D Fe_nGeTe_2 (n=3-5) magnets with van der Waals (vdW) stacked layers has attracted enormous attention due to high Curie temperatures and the potential of use in spintronic applications. The possibility of tunability in structural, electronic and magnetic properties has been instrumental in achieving novel properties in these 2D magnets and their heterostructures. Furthermore, recent experimental studies have revealed unusual magnetic phenomena by doping with Ni or Co in Fe_5GeTe_2 in particular, which calls for detailed quantitative analysis. In this presentation, with the aid of first principles theory, a systematic evolution of magnetic exchange interactions and Curie temperatures with Ni doping will be demonstrated. The microscopic mechanisms will be presented as an interplay between specific magnetic exchange interactions, magnetic anisotropy and Dzyaloshinskii-Moriya interactions. Moreover, the role of dynamical correlation will be highlighted via the study with dynamical mean field theory. The case of Co doping will be highlighted to explain the magnetic anisotropy change due to doping via the analysis of atom and orbital resolved magnetic anisotropy energies. For both the cases with Co and Ni doping, our results are in good agreement with the experimental observations.

MA 29.12 Wed 18:00 EB 202

Evolution of van der Waals gap and exchange bias in $Fe_3GeTe_2/MnPS_3$ vdW heterostructure — Aravind Puthirath Balan[1], •Aditya Kumar[1], Patrick Reiser[2], Joseph Vimal Vas[3], Thibaud Denneulin[3], Andras Kovacs[3], Patrick Maletinsky[2], and Mathias Kläui[1] — [1]Institute of Physics, Johannes Gutenberg University Mainz, Staudinger Weg 7, 55128 Mainz, Germany — [2]Department of Physics, University of Basel, Klingelbergstrasse 82, 4056 Basel, Switzerland — [3]Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons and Peter Grünberg Institute, Forschungszentrum Jülich, 52425 Jülich, Germany

The inherent layered structure of Van der Waals (vdW) materials allows the fabrication of heterostructures with perfect interfaces and the study of interface-related phenomena such as Exchange bias (EB) [1]. This study presents a comprehensive analysis of EB in the Fe_3GeTe_2 (FM) and $MnPS_3$ (AFM) vdW heterostructure, revealing insights into its origin and unique evolving nature. A large EB of 170 mT was observed at 5K in this system due to pinning from anomalous ferromagnetic ordering that emerges in $MnPS_3$ at low temperatures. The evolving nature of EB is due to thermal cycling-induced modification of the interface registry, accompanied by vdW gap modification, as confirmed by STEM measurements. This work offers new insights into the nature of interfaces between vdW materials and the potential method for tuning EB and the vdW gap.

[1] Balan et al. arXiv preprint arXiv:2303.13167 (2023)

MA 29.13 Wed 18:15 EB 202

Hyperfine interactions in open-shell planar sp^2-carbon nanostructures — Sanghita Sengupta[1], Thomas Frederiksen[1,2], and •Géza Giedke[1,2] — [1]Donostia International Physics Center (DIPC), E-20018, Donostia-San Sebastián, Spai — [2]IKERBASQUE, Basque Foundation for Science, E-48013, Bilbao, Spain

We investigate hyperfine interaction (HFI) using density-functional theory for several open-shell planar sp^2-carbon nanostructures displaying π magnetism such as $[n]$triangulenes and graphene nanoribbons. Our results indicate that HFI can reach 100 MHz and that isotropic Fermi contact and anisotropic dipolar terms contribute in comparable strength, rendering the HFI markedly anisotropic. Using these results we obtain empirical models using generic sp^2-HFI fit parameters that connect the HFI to the π-spin polarizations at carbon sites only. These models successfully describe the Fermi contact and dipolar contributions for 13 C and 1 H nuclei and allow to obtain hyperfine tensors for large systems where existing methodology is not suitable or computationally too expensive. Implications of the obtained HFI for electron-spin decoherence, dynamical nuclear polarization, and for coherent nuclear dynamics are discussed.

MA 29.14 Wed 18:30 EB 202

Magnetic ordering in weakly coupled van der Waals systems — •Karel Carva and Krishna K. Pokhrel — Charles University, Faculty of Mathematics and Physics, DCMP, Ke Karlovu 5, 121 16 Prague 2, Czech Republic

Magnetic van der Waals materials exhibit promising potential for high-tech magnetic applications in nanostructures [1]. Their weak interlayer coupling leads to magnetic behavior different from the more explored cases of isotropic bulk-like exchange or the ideal 2D (monolayer) limit [2]. Here we examine general features of finite temperature magnetic order in this regime by atomistic spin dynamics methods. The method is applied to a particularly interesting system from this class, VI_3. Its anisotropy was reproduced by first-principles calculations only if lattice distortions present at its low temperature phases were taken into account [3]. The calculations also revealed an exceptionally large orbital momentum on V atoms; these findings are compared to recent measurements based on the x-ray magnetic circular dichroism [4]. Employing calculated exchange interactions we study how is the Curie temperature affected by interlayer coupling in this system.

[1] K. Burch, et al., Nature 63 (2018) 47
[2] V. Y. Irkhin, A. A. Katanin, and M. I. Katsnelson, Phys. Rev. B 60 (1999) 1082
[3] L. M. Sandratskii and K. Carva, Phys. Rev. B 103 (2021) 214451
[4] D. Hovančík et al., Nano Lett. 23 (2023) 1175

MA 29.15 Wed 18:45 EB 202

Emergent altermagnetism: magnetically induced anomalous Hall conductivity — •Toshihiro Sato[1], Sonia Haddad[2], Ion Cosma Fulga[1], Fakher F. Assaad[3,4], and Jeroen van den Brink[1,4,5] — [1]Institute for Theoretical Solid State Physics, IFW Dresden, Germany — [2]Laboratoire de Physique de la Matière Condensée, Faculté des Sciences de Tunis, Université Tunis El Manar, Tunisia — [3]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Germany — [4]Würzburg-Dresden Cluster of Excellence ct.qmat, Germany — [5]Institut für Theoretische Physik, Technische Universität Dresden, Germany

We introduce a novel model that demonstrates the emergence of altermagnetism driven by electron interactions. This model is grounded in a spin-full modified Haldane framework, where electron interactions play a crucial role. Employing quantum Monte Carlo simulations, we successfully demonstrate the emergence of an altermagentic phase. This phase exhibits spontaneously time-reversal symmetry-broken antiferromagnetic order and is characterized by spin-split bands without a net magnetic moment. Moreover, a significant observation is the simultaneous emergence of an anomalous quantum Hall order alongside this antiferromagnetic order. The concurrent appearance of both orders results in a measurable, finite anomalous Hall conductivity.