MA 21: Spin-Dependent Phenomena in 2D

Time: Tuesday 15:00–17:15 Location: HSZ 403

MA 21.1 Tue 15:00 HSZ 403

Material design of topological magnetism in 2D heterostructures — •Nihad AbuAwwad[1,2], Manuel dos Santos Dias[3], and Samir Lounis[1,2] — [1]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich & JARA, 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 discovery of two-dimensional (2D) van der Waals magnetic materials and their heterostructures provided an exciting platform for emerging phenomena with intriguing implications in information technology. $CrTe_2$ is a particular example that hosts complex magnetism strongly intertwined with its crystal structures [1,2]. Here, based on a multiscale modelling approach that combines first-principles calculations and a Heisenberg model, we demonstrate that interfacing this 2D layer with various Te-based layers hosting heavy or light elements enables the control of the Dzyaloshinskii-Moriya interaction and magnetic anisotropy energy of the whole heterostructure, and thereby the emergence of new magnetic phases of matter, which are of topological nature such as skyrmions and merons.

–Work funded by the Palestinian-German Science Bridge (BMBF–01DH16027) and Priority Programme SPP 2244 2D Materials Physics of van der Waals Heterostructures of the DFG (project LO 1659/7-1).

[1] AbuAwwad *et al.*, J. Phys.: Condens. Matter **34**, 454001(2022).
[2] Xian *et al.*, Nat. Commun. **13**, 257 (2022).

MA 21.2 Tue 15:15 HSZ 403

Tuning the magnetic interactions in van der Waals Fe_3GeTe_2 heterostructures — Dongzhe Li[1], •Soumyajyoti Haldar[2], Tim Drevelow[2], and Stefan Heinze[2] — [1]CEMES, Université de Toulouse, CNRS, 29 rue Jeanne Marvig, F-31055 Toulouse, France — [2]Institute of Theoretical Physics and Astrophysics, University of Kiel, Leibnizstrasse 15, 24098 Kiel, Germany

We investigate the impact of mechanical strain, stacking order, and external electric fields on the magnetic interactions of a Fe_3GeTe_2 monolayer deposited on Germanene using density functional theory [1]. We find that an electric field of $\mathcal{E} = \pm 0.5$ V/Å applied perpendicular to the Fe_3GeTe_2/germanene heterostructure leads to significant changes of the exchange constants. We show that the Dzyaloshinskii-Moriya interaction (DMI) in Fe_3GeTe_2/Germanene is mainly dominated by the nearest neighbors. Furthermore, we demonstrate that the DMI is highly tunable by strain, stacking, and electric field, leading to a large DMI comparable to that of ferromagnetic/heavy metal interfaces. The geometrical change and hybridization effect explain the origin of the high tunability of the DMI at the interface. The magnetocrystalline anisotropy energy (MAE) can also be drastically changed by the application of compressive or tensile strain. The tunability of DMI and MAE by using strain allows the occurrence of nanoscale skyrmions [2].

[1] D. Li, S. Haldar, T. Drevelow, S. Heinze, arXiv:2210.15351.
[2] D. Li, S. Haldar, S. Heinze, Nano Lett. **22**, 7706 (2022).

MA 21.3 Tue 15:30 HSZ 403

Spin-texture of graphene on Co films on heavy metals — •Donya Mazhjoo[1,2], Gustav Bihlmayer[1], and Stefan Blügel[1] — [1]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany — [2]Physics Department, RWTH-Aachen University, 52062 Aachen, Germany

Graphene(Gr) covered ferromagnetic films deposited on heavy metals (HM) have been proposed for the exploration of novel spin-orbitronic devices since they possess a perpendicular magnetic anisotropy (MA) as well as a sizable Dzyaloshinskii-Moriya interaction (DMI). By using density functional theory as implemented in the Fleur-code [1], we investigate the spin-orbit (SO) induced spin-texture of Gr covered Co/Ir(111) heterostructures. We consider SOC in first order perturbation theory to study the DMI and self-consistently for the MA energy. Various thicknesses of Co are investigated and compared to experimental data. There, for thin Co films, spin- and angular-resolved photoemission spectroscopy found an in-plane spin-polarization of the Gr π bands, consistent with a HM induced Rashba-type SO coupling at the Gr/Co interface [2]. We compare to Pt(111) as HM substrate looking for signatures of the DMI in the (induced) spin-textures.

Support from the FLAG-ERA JTC 2019 grant SOgraphMEM is gratefully acknowledged.

[1] https://www.flapw.de
[2] B. Cano et al. arXiv:2206.04351

MA 21.4 Tue 15:45 HSZ 403

Magnetism and THz excitations in quasi-2D systems perturbed by external fields — •Karel Carva and Krishna K. Pokhrel — Charles University, Faculty of Mathematics and Physics, DCMP, Ke Karlovu 5, 121 16 Prague 2, Czech Republic

Systems with a very weak exchange coupling between magnetically ordered layers represent an interesting intermediate stage between the well-known isotropic bulk magnets and the recently intensively studied 2D magnets [1]. We perform a complex investigation of lattice and magnetic excitations induced by external perturbations in such quasi-2D system, trihalide VI_3, employing the synergy of DFT calculations, infrared, THz, and Raman spectroscopies [2]. The transition to the long-range ferromagnetic order is accompanied by the observed variations of phonon frequencies indicating strong magnetoelastic coupling. The acoustic magnon mode acquires here unusually high energy reaching to the THz range, but dramatically softens at temperatures where a second lattice distortion has been reported. First-principles calculations also show the strong connection of magnetic ordering and anisotropy to the lattice and its low temperature distortions [3]. These findings suggest the possibility of controlling magnetic anisotropy in this system by selective occupation of specific lattice modes. In this way magnon spectra would be strongly modified as well. We also show changes induced by strong magnetic fields in VI_3 and similar systems.

[1] M. Gibertini et al., Nat. Nanotech. 14, 408 (2019)
[2] D. Hovančík et al., J. Phys. Chem. Lett. 13, 11095 (2022)
[3] L. M. Sandratskii, K. Carva, Phys. Rev. B 103, 214451 (2021)

15 min. break

MA 21.5 Tue 16:15 HSZ 403

Characterisation of the Ising-tye 2D magnet $FePS_3$: A DFT+U study — Mohammad Amirabbasi and •Peter Kratzer — Faculty of Physics, University Duisburg-Essen, 47057 Duisburg, Germany

Among the 2D magnetic system that can be prepared via exfoliation, iron phosphorus trisulfide ($FePS_3$) excels due to its unusual Ising-type magnetic order which makes it interesting for applications in spintronic nano-devices. We carried out a computational study of the structural and magnetic properties of single-layer $FePS_3$ by using Density Functional Theory (DFT+U). Our findings show that the sublattice of the Fe^{2+} ions is not a perfect honeycomb; rather the nearest-neighbor Fe distances vary by 0.14 Å as a result of orbital ordering. These lattice distortions, albeit small, trigger different (ferromagnetic and antiferromagnetic) exchange couplings so that the ground state consists of ferromagnetically aligned zig-zag chains along the long Fe-Fe bonds which couple antiferromagnetically along the shorter Fe-Fe bonds of the distorted honeycomb. Within the DFT+U framework, we parameterize a spin Hamiltonian including Heisenberg, single-ion anisotropy, Dzyaloshinskii-Moriya and biquadratic interactions that allows us to calculate the critical temperature and the magnon spectrum. By comparing to prior results from neutron scattering, we conclude that it is the upper magnon branch in a doubled unit cell that has been observed in these experiments.

MA 21.6 Tue 16:30 HSZ 403

Interaction parameters in magnetic 2D systems from symmetric invariants — •Jonathan Kipp[1,2], Yuriy Mokrousov[2,3], and Fabian R. Lux[3] — [1]Department of Physics, RWTH Aachen University, 52056 Aachen, Germany — [2]Institute for Advanced Simulation, Forschungszentrum Jülich Wilhelm-Johnen-Straße, 52428 Jülich — [3]Institute of Physics, Johannes Gutenberg University Mainz, 55099 Mainz, Germany

The electronic properties of 2D materials hosting complex magnetic order can have crucial implications for information storage and processing applications. At the heart of the complexity in these materials is the interplay of external fields, fluctuations and electronic structure

with the magnetic properties. In this work, we are aiming to uncover the direct implications that changes in the magnetic texture have on the electronic characteristics of the system. We develop an expansion in terms of the textures symmetric invariants and compare to data obtained from Heisenberg Hamiltonians, tight-binding (TB) calculations or possibly even density functional theory (DFT) calculations by employing a machine learning (ML) algorithm for the fitting task. Specifically, this enables us to identify the relevant interaction terms from the expansion to the total energy, since there is a diverse palette of ML fitting algorithms aiming at sparse models with the smallest possible number of coefficients, including regularized and sequential approaches.

MA 21.7 Tue 16:45 HSZ 403

Locally driven quantum phase transition cascades in a strongly correlated molecular monolayer — Soroush Arabi[1,2,3], Taner Esat[2,5], Aizhan Sabitova[2,5], Yuqi Wang[2,3], Hovan Lee[7], Cedric Weber[7], Klaus Kern[3,4], F. Stefan Tautz[1,2,5], Ruslan Temirov[2,6], and •Markus Ternes[1,2,5] — [1]Institute of Physics IIB, RWTH Aachen University, 52074 Aachen, Germany — [2]Peter-Grünberg-Institute (PGI 3), Research Center Jülich, 52425 Jülich, Germany — [3]Max Planck Institute for Solid State Research, 70569 Stuttgart, Germany — [4]Institut de Physique, École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland — [5]Jülich Aachen Research Alliance, 52425 Jülich, Germany — [6]Institute of Physics II, University of Cologne, 50937 Cologne, Germany — [7]King's College London, Theory and Simulation of Condensed Matter, London WC2R 2LS, UK

The molecular monolayer of 1,4,5,6-naphthalene tetracarboxylic acid dianhydride on Ag(111) creates a perfectly ordered lattice of π-conjugated organic molecules. Using a movable atomically sharp electrostatic gate we drive this lattice of strongly correlated electrons through a cascade of quantum phase transitions. Performing spectroscopic imaging with sub-Angstrom resolution, we show that as the gate field is increased, the molecular building blocks change from a Kondo-screened to a paramagnetic phase one by one, enabling us to reconstruct their complex interactions in detail. We anticipate that the supramolecular nature of the system will, in future, allow engineering quantum correlations in arbitrary patterned structures.

MA 21.8 Tue 17:00 HSZ 403

Electrically Tunable Curie Temperature in a 2D Ferromagnetic Semiconductor — •Tania Mukherjee[1,2] and Soumya Jyoti Ray[1] — [1]Department of Physics, Indian Institute of Technology Patna, Bihta 801106, India — [2]Institute of Optics and Atomic Physics, Technical University of Berlin, Straße des 17. Juni 135, 10623 Berlin, Germany

Magnetic van der Waal's nanocrystals with intrinsic magnetic anisotropy provide an ideal platform for exploring magnetism in the low-dimensional limit. We investigate the electronic and magnetic properties of a novel 2D material $VClBr_2$ by using spin polarised density functional theory calculations. We observe complex electronic and magnetic phase transitions, tunable bandgap, and extremely large enhancement of the Curie temperature under the application of strain (η) and electric field (Ez). A Monte Carlo approach to the resolution of the Ising model reveals that the Curie temperature (T_c) can reach up to 340K under the application of an $E_z = 2.5$ V/nm, a colossal enhancement of $\sim$ 6700% of its base value. The coexistence of high-temperature spin-ordering along with large magnetic anisotropic energy (MAE), high magnetic moment, tunable band gap, and excellent stability make single layer $VClBr_2$ a promising material for applications in an electric field driven spin gating, room temperature spintronics, and 2D spin circuit design.