MA 46: Poster II

Time: Thursday 15:00–18:00 Location: Poster C

MA 46.1 Thu 15:00 Poster C

Interface driven emergent electromagnetic induction in $SrRuO_3$/$SrIrO_3$-bilayers — •Ludwig Scheuchenpflug[1], Robert Gruhl[1], Sebastian Esser[2], and Philipp Gegenwart[1] — [1]Experimentalphysik VI, Universität Augsburg, Germany — [2]Department of Applied Physics, University of Tokyo, Japan

Recently, emergent electromagnetic induction (EEMI), induced through current driven spin dynamics, was predicted [1] and later observed in the spin-helix magnet $Gd_3Ru_4Al_{12}$ [2] opening a new direction for material research and paving the way towards further miniaturisation of elements for electrical circuits.

Bilayers of ferromagnetic $SrRuO_3$ and paramagnetic $SrIrO_3$ display a topological Hall effect (THE) which was related to the formation of Néel-skyrmions arising from the Dzyaloshinskii-Moriya interaction at the interface [3,4]. Such skyrmions could also show the EEMI effect. We fabricated bilayers of $SrRuO_3$/$SrIrO_3$ on $SrTiO_3$ (001) substrates by metal-organic aerosol deposition and confirmed their quality with X-ray diffraction and TEM imaging. Besides Hall measurements, precise impedance measurements are analyzed at several temperatures and frequencies on a variety of microstructured samples.

[1] N. Nagaosa, Jpn. J. Appl. Phys. 58, 120909 (2019).
[2] Yokouchi et al., Nature 586, s41586-020-2775-x (2020).
[3] J. Matsuno et al., Science Adv. 2, e1600304 (2016).
[4] S. Esser et al., Phys. Rev. B 103, 214430 (2021).

MA 46.2 Thu 15:00 Poster C

Skyrmion flow in a periodically modulated channel — •Klaus Raab, Maurice Schmidt, Maarten A. Brems, Jan Rothörl, Fabian Kammerbauer, Peter Virnau, and Mathias Kläui — Institut für Physik, Johannes Gutenberg-Universität Mainz, Staudingerweg 7, 55128 Mainz, Germany

We investigate the non-equilibrium flow behaviour of skyrmions, magnetic whirls with non-trivial real space topology, driven by spin-torques in modulated channel geometries. Poiseuille-like velocity flow-profiles of liquids usually occur due to no-slip boundary conditions, meaning moving particles do interfere with the boundary e.g. the wall of the confining geometry, reducing the velocity of particles closest to a wall1. Skyrmions on the other hand should experience slip at the boundaries due to the repulsive nature of the skyrmion-edge and skyrmion-skyrmion interaction. Adding structured obstacles along the boundary may lead to partial or even no-slip behaviour and thus to Poiseuille-like flow profiles while skyrmions are forced through a wire due to spin-torques. Influence of channel width and edge geometry modulation were optimized and tested using simulations and compared with experimental measurements of straight and modulated channels. Understanding flow dynamics and velocity profiles of skyrmions, their interaction with each other and their harbouring geometry is essential for skyrmionic applications like the racetrack memory2. 1. Sutera, S. P. & Skalak, R. The History of Poiseuille*s Law. Annu. Rev. Fluid Mech. 25, 1-20 (1993). 2. Fert, A., Cros, V. & Sampaio, J. Skyrmions on the track. Nat. Nanotechnol. 8, 152-156 (2013).

MA 46.3 Thu 15:00 Poster C

Manipulating magnetic textures with scanning local magnetic field — •Minh Duc Tran and Mathias Kläui — Institute of Physics, Johannes Gutenberg University Mainz, 55099 Mainz, Germany

We demonstrate local manipulation of magnetic textures in CoFeB/MgO multilayers based on the interaction between the sample and a customized magnetic force microscopy probe. By varying the scan height, write speed, number of scans, and specific magnetic coating of the tip, a tunable local stray field can induce desirable manipulation of the magnetic system. Complex topological textures such as skyrmions can be nucleated and manipulated individually, either by collapsing the stripe domains or cutting them into skyrmions with the aid of an external magnetic field [1]. Our results offer deterministic control of a skyrmion at a localized area, which can be beneficial, for instance, in future applications in skyrmion racetrack memory [2].

[1] A. V. Ognev et al., ACS Nano 14, 11, 14960-14970 (2020).
[2] A. Casiraghi et al., Commun. Phys. 2, 145 (2019).

MA 46.4 Thu 15:00 Poster C

Gesture recognition with Brownian reservoir computing using geometrically confined skyrmion dynamics — •Grischa Beneke[1], Thomas Brian Winkler[1], Klaus Raab[1], Maarten Brems[1], Fabian Kammerbauer[1], Johan Mentink[2], and Mathias Kläui[1] — [1]Institut für Physik, Johannes Gutenberg-Universität Mainz, Germany — [2]Radboud University, Institute for Molecules and Materials, The Netherlands

Physical Reservoir Computing (RC) represents a significant advance for reducing the training time and energy consumption in non-conventional computing. It has been shown that magnetic skyrmions, topological particle-like spin textures, are promising candidates for unconventional computing [2,3] due to their non-linear interactions and efficient mechanisms for manipulation. Leveraging the thermally activated diffusive motion [2] and utilizing an automatic reset mechanism prompted by the repulsion of skyrmions from magnetic material boundaries has facilitated the realization of spatially multiplexed RC [3]. Here we take the next step and realize time-multiplexed RC. We present a hardware-based approach to distinguish various hand gestures captured via a Doppler radar, involving the application of a time-varying voltage to observe and track the trajectory of skyrmions. Notably, our device exhibits competitive performance when compared to an energy intensive approach [4]. [1] D. Gauthier et al., Nat. Comms. 12, 5564 (2021). [2] J. Zázvorka et al., Nat. Nanotechnol. 14, 658 (2019). [3] K. Raab et al., Nat. Comms. 13, 6982 (2022). [4] G. Beneke et al., in preparation (2023).

MA 46.5 Thu 15:00 Poster C

Direct observation of Néel-type skyrmions and domain walls in a ferrimagnetic DyCo3 thin film — •Chen Luo[1,2], Kai Chen[1,3], Victor Ukleev[1], Sebastian Wintz[1,4], Markus Weigand[1,4], Radu-Marius Abrudan[1], Karel Prokeš[1], and Florin Radu[1] — [1]Helmholtz-Zentrum-Berlin für Materialien und Energie, Albert-Einstein-Straße 15, 12489, Berlin, Germany — [2]Institute of Experimental Physics of Functional Spin Systems, Technical University Munich, James-Franck-Straße 1, 85748, Garching b München, Germany — [3]National Synchrotron Radiation Laboratory, University of Science and Technology of China, 230029, Hefei, Anhui, China — [4]Max-Planck-Institut für Intelligente Systeme, 70569, Stuttgart, Germany

Isolated magnetic skyrmions are at the forefront of research interests due to their potential applications in information technology. A distinct class of skyrmion hosts are rare earth - transition metal (RE-TM) ferrimagnetic materials. We report on an ferrimagnetic material DyCo3 with a strong perpendicular anisotropy, the ferrimagnetic skyrmion size can be tuned by an external magnetic field. By taking advantage of the scanning transmission X-ray microscopy and utilizing a large x-ray magnetic linear dichroism contrast that occurs naturally at the RE resonant edges, we resolve the nature of the magnetic domain walls of ferrimagnetic skyrmions. We demonstrate that through this method one can easily discriminate between Bloch and Néel type domain walls for each individual skyrmion. For all isolated ferrimagnetic skyrmions, we observe that the domain walls are of Néel-type.

MA 46.6 Thu 15:00 Poster C

Chiral surface spin textures in Cu_2OSeO_3 unveiled by soft x-ray scattering in specular reflection geometry — •Victor Ukleev[1], Chen Luo[1], Radu Abrudan[1], Aisha Aqeel[2], Christian Back[2], and Florin Radu[1] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany — [2]Physik-Department, Technische Universität München, Garching, Germany

Resonant elastic soft x-ray magnetic scattering (XRMS) is a powerful tool to explore long-periodic spin textures in single crystals. However, due to the limited momentum transfer range imposed by long wavelengths of photons in the soft x-ray region, Bragg diffraction is restricted to crystals with the large lattice parameters. Alternatively, small angle x-ray scattering has been involved in the soft energy x-ray range which, however, brings in difficulties with the sample preparation that involves focused ion beam milling to thin down the crystal to below a few hundred nm thickness. We show how to circumvent these restrictions by using XRMS in specular reflection from a sub-nanometer smooth crystal surface. The method allows observing diffraction peaks from the helical and conical spin modulations at the

surface of a Cu_2OSeO_3 single crystal and probing their corresponding chirality as contributions to the dichroic scattered intensity. The results suggest a promising way to carry out XRMS studies on plethora of noncentrosymmetric systems hitherto unexplored with soft x-rays due to the absence of the commensurate Bragg peaks in the available momentum transfer range [1]. [1] Ukleev, V., et al., Sci. Technol. Adv. Mater. 23, 683 (2022).

MA 46.7 Thu 15:00 Poster C

Coarse-Grained Computer Simulations of Skyrmions — •Simon Fröhlich, Jan Rothörl, Maarten A. Brems, Tobias Sparmann, Raphael Gruber, Mathias Kläui, and Peter Virnau — Institute of Physics, Johannes Gutenberg Universität, Mainz, Deutschland

Magnetic skyrmions are often described as 2D quasi-particles governed by the Thiele equation [1]. This abstraction allows for simulations of a large number of skyrmions on experimentally relevant time scales [2]. To accurately describe the experimental behavior, we determine an effective interaction potential [3] as well as a description of skyrmion pinning [4]. We will also discuss first ideas for matching experimental and simulation time scales to capture real dynamics in quasi-particle simulations.

[1] A. A. Thiele, Phys. Rev. Lett. 30, 230 (1973)
[2] J. Zázvorka et al., Adv. Funct. Mater, 30, 2004037 (2020)
[3] Y. Ge et al., Commun. Phys. 6, 30 (2023)
[4] R. Gruber et al., Nat. Commun. 13, 3144 (2022)

MA 46.8 Thu 15:00 Poster C

Magnetic anisotropy and anisotropic critical fields in MnSi and $Fe_{1-x}Co_xSi$ — •Gilles Gödecke, Julius Grefe, Stefan Süllow, and Dirk Menzel — Institut für Physik der Kondensierten Materie, TU Braunschweig, Mendelssohnstr.3, 38106 Braunschweig, Germany

The itinerant B20 bulk magnets MnSi and $Fe_{1-x}Co_xSi$ are known to host chiral spin structures and magnetic skyrmions arising from competing magnetic interactions including magnetic anisotropy. We report on the measurement of the magnetic anisotropy constants for MnSi and $Fe_{1-x}Co_xSi$ ($0.08 \leq x \leq 0.30$) using angle-resolved magnetisation measurements in a commercial SQUID magnetometer. From the measurements, we have identified the angle dependence of the critical fields H_{C1} and H_{C2}. Whereas both H_{C1} and H_{C2} for MnSi are maximal along the hard axis, the behavior of H_{C1} is opposite for $Fe_{1-x}Co_xSi$. The values of the anisotropy constants at $T = 5$ K are $K = -12 \times 10^2$ J/m^3 for MnSi and $K = (2...6) \times 10^2$ J/m^3 for $Fe_{1-x}Co_xSi$.

MA 46.9 Thu 15:00 Poster C

Determining pinning influence on skyrmion diffusion in 2D — •Tobias Sparmann, Simon Fröhlich, Jan Rothörl, Maarten A. Brems, Fabian Kammerbauer, Peter Virnau, and Mathias Kläui — Department of Physics, Johannes-Gutenberg University Mainz

Magnetic skyrmions are considered potential candidates for the development of probabilistic computing devices since they respond strongly nonlinearly to external stimuli and feature inherent multiscale dynamics [1].

The implementation of this type of probabilistic computing relies on thermal excitation and diffusive motion of the magnetic skyrmions within thin films, which exhibit pinning due to sample inhomogeneities [2]. To better understand the impact of pinning on larger scales, we need to model and understand the effective energy landscape of all areas the skyrmion can inhabit [3].

In this work, we investigate the spatial and temporal resolution limits we hit when determining the exact effective energy landscape, and we have a closer look at the specific characteristics of skyrmion diffusive motion. With this, we develop methods to overcome those limits and end up with a complete energetic model of skyrmion pinning and diffusion [4].

[1] D. Prychynenko et al., Phys. Rev. Applied, 9, 014034 (2018).
[2] J. Zázvorka et al., Nat. Nanotechnol., 14, 658 (2019).
[3] R. Gruber et al., Nat. Commun., 13, 3144 (2022).
[4] T. Sparmann et al., in preparation (2023).

MA 46.10 Thu 15:00 Poster C

Room Temperature Skyrmions in Pt/Co/Ta multilayers — Liz Montañez[1], Emmanuel Kentzinger[2], David Cortie[3], Valentin Ahrens[4], Laura Guasco[5], Thomas Keller[5], Markos Skoulatos[6], Markus Becherer[4], and •Sabine Pütter[1] — [1]FZ Jülich, Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Garching, Germany — [2]FZ Jülich, JCNS and Peter Grünberg Institut, JARA-FIT, Germany — [3]ARC Centre of Excellence in Future Low Energy Electronics Technologies and Institute for Superconducting and Electronic Materials, University of Wollongong, Australia — [4]Chair of Nano and Quantum Sensors, TU of Munich, Germany — [5]Max Planck Society Outstation at the MLZ, Garching, Germany — [6]MLZ and Physics Department, TU of Munich, Germany

Magnetic skyrmions are topologically stabilized spin configurations on the nanoscale. In magnetic multilayers, they can be stabilized at room temperature. Polycrystalline[Pt(40Å)/Co(x)/Ta(19Å)]$_N$ multilayers were fabricated in a molecular beam epitaxy setup by thermal deposition on oxidized Si(001) substrates with a Ta buffer layer and a Pt cap layer. The Co film thickness was varied between 5 Å and 21 Å and N varied between 8 and 10.

Magnetic force microscopy measurements reveal the existence of skyrmions at a Co thickness between 9 Å and 17 Å. We discuss results obtained from magnetic hysteresis, transport and neutron reflectometry measurements. The latter have been performed with the neutron reflectometer Platypus at ANSTO, Australia.

MA 46.11 Thu 15:00 Poster C

Skyrmion dynamics in the stripe domain phase — •Omer Fetai[1], Lisa-Marie Kern[2], Ross Knapman[1,3,4], Maike L. Auer[2], Bastian Pfau[2], and Karin Everschor-Sitte[1,4] — [1]TWIST Group, University of Duisburg-Essen, Duisburg, Germany — [2]Max-Born-Institut, Berlin, Germany — [3]Johannes Gutenberg University Mainz, Mainz, Germany — [4]Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, Duisburg, Germany

The skyrmion Hall effect, which deflects skyrmions from the direction of the driving electric current, is a major challenge for racetrack-like applications. Guiding the skyrmion motion and suppressing the skyrmion Hall effect is possible by modifying the energy landscape of the skyrmion-carrying racetrack. This can, for example, be achieved by ion irradiation [1], where the material properties are engineered. Alternatively, skyrmions can be embedded in a stripe domain phase such that the magnetic texture itself induces tracks along which the skyrmions move straight [2-4]. We combine the ideas of skyrmions embedded in stripe domain phases with tailored properties and investigate the skyrmion dynamics under the influence of Spin-Orbit-Torques. [1] Kern et al., Nano Lett. 2022, 22, 10, 4028*4035 [2] Müller, et al. Phys. Rev. Lett. 119, 137201 (2017) [3] Knapman et al., J. Phys. D: Appl. Phys. 54 404003 (2021) [4] Song et al., arXiv:2212.08991 (2022)

MA 46.12 Thu 15:00 Poster C

Current driven skyrmion movement and their electrical detection in Ta/CoFeB/MgO — •Hauke Lars Heyen[1], Malte Römer-Stumm[2], Jakob Walowski[1], Christian Denker[1], Kornel Richter[2], Jeffrey McCord[2], and Markus Münzenberg[1] — [1]Institute for Physics, University Greifswald, Germany — [2]Institute for Materials Science, Nanoscale Magnetic Materials and Magnetic Domains, CAU Kiel, Germany

Magnetic skyrmions are two-dimensional topological protected round spin structures. They have a strong potential for application in future storage devices like the conceptual skyrmion race-track memory. Such an implementation requires fundamental control over the dynamics of skyrmion motion and reliable tools for their detection. Skyrmions can be generated in Ta/CoFeB/MgO layer stacks at room temperature. Nanosecond electric current pulses on the nanosecond scale enable relocating the skyrmions using current densities from 10^12 - 10^13 A/m^2. The dynamic trajectories hint at the skyrmion-Hall effect and superdiffusion. The skyrmion-Hall effect results from the skyrmion topology, and the superdiffusion occurs due to defects on the motion path. Magnetic tunnel junctions (MTJ) are a promising tool to detect small magnetization changes. The selected Ta/CoFeB/MgO material system allows integrating MTJs into skyrmion samples. However, this integration of MTJs remains challenging, even though they work fine independently.

MA 46.13 Thu 15:00 Poster C

Room-Temperature Skyrmions in Ir/Fe/Co/Pt Multilayers Coupled to Co/Pt Multilayers — •Joe Sunny, Timo Schmidt, Tamer Karaman, and Manfred Albrecht — Institute of Physics, University of Augsburg, D-86159 Augsburg, Germany

Magnetic skyrmions are topologically protected swirling magnetic spin

structures which can be stabilized by Dzyalonshinskii-Moriya interactions (DMI). In recent years, considerable research efforts have been dedicated to stabilizing and manipulating skyrmions at room temperature in multilayer systems as these promise applications in skyrmion-based topological spintronics. The system studied combined of a skyrmion hosting multilayer of Ir/Fe/Co/Pt and a ferromagnetic layer of Co/Pt with perpendicular easy axis of magnetization separated by a non-magnetic spacer layer of Cu. The skyrmion layer hosts skyrmions of Néel-type stabilized by the interlayer DMI from the Ir/Fe and Co/Pt interfaces[1]. The magnetic domains formed in the skyrmion hosting layer are coupled to the ferromagnetic layer via the Cu spacer by Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction. From the Lorentz transmission electron microscope (LTEM) imaging the spin objects are observed to be not entirely Néel-type but also have a Bloch-type contrast. To study if the skyrmions from the underlying layer are completely imprinted onto the top Co/Pt layer, X-ray magnetic circular dichroism (XMCD) measurements were performed.

References

1.Anjan Soumyanarayanan et.al, Nature Mater 16, 898*904 (2017).

MA 46.14 Thu 15:00 Poster C

Engineering of Néel-type Skyrmions in Novel Freestanding Heterostructures — •Zihan Yin, Peng Wang, Ke Gu, Abhay Srivastava, and Stuart Parkin — Max Planck Institute of Microstructure Physics, Halle, Germany

Skyrmions are spatially inhomogeneous spin textures with nanoscale size. Néel-type skyrmions can be induced by interfacial symmetry broken. They are regarded as novel information carriers for use in high-density, low-power, and multi-functional spintronic devices. In this project, we use freestanding technology to tune the strain effects in ferromagnets. The phase of spin textures can be observed through Lorentz Transmission Electron Microscope (LTEM).

In this project, the wrinkles on the freestanding heterostructure thin film can result in various types of magnetic textures due to the varying strain. And with applied field, we can observe difference in density for both strip and skyrmion phase.

MA 46.15 Thu 15:00 Poster C

Skyrmion Stripes in Twisted Double Bilayer Graphene — •Debasmita Giri[1,2], Dibya Kanti Mukherjee[3,4], Herbert A. Fertig[4,5,6], and Arijit Kundu[2] — [1]University of Regensburg, Regensburg, Germany — [2]Department of Physics, Indian Institute of Technology Kanpur, Kanpur 208016, India — [3]Laboratoire de Physique des Solides, CNRS UMR 8502, Universitè Paris-Saclay, 91405 Orsay Cedex, France — [4]Department of Physics, Indiana University, Bloomington, IN 47405 — [5]Quantum Science and Engineering Center, Indiana University, Bloomington, IN, 47408 — [6]Instituto de Ciencia de Materiales de Madrid, (CSIC), Cantoblanco, 28049, Madrid, Spain

Two-dimensional moiré systems have recently emerged as a platform in which the interplay between topology and strong correlations of electrons play out in non-trivial ways. Among these systems, twisted double bilayer graphene (TDBG) is of particular interest as its topological properties may be tuned via both twist angle and applied perpendicular electric field. In this system, energy gaps are observed at the half-filling of particular bands, which can be associated with correlated spin-polarized states. In this work, we investigate the fate of these states as the system is doped away from this filling. We demonstrate that, for a broad range of fractional fillings, the resulting ground state is partially valley polarized and supports multiple broken symmetries, including a textured spin order indicative of skyrmions, with a novel stripe ordering that spontaneously breaks C3 symmetry.

MA 46.16 Thu 15:00 Poster C

Cavity-based excitation of Magnetization dynamics in a skyrmion host material — •Philipp Schwenke[1], Lars Hess[1], Ephraim Spindler[1], Aisha Aqeel[2], Vitaliy Vasyuchka[1], Christian Back[2], and Mathias Weiler[1] — [1]Fachbereich Physik and Landesforschungszentrum OPTIMAS, Rheinland-Pfälzische Technische Universität Kaiserslautern-Landau, 67663 Kaiserslautern, Germany — [2]Physik-Department, Technische Universität München, 85748 Garching, Germany

Magnetic skyrmions are vortex-like topologically protected spin textures that typically occur in chiral magnets with Dzyaloshinskii-Moriya interactions. A prominent skyrmion host material is Cu_2OSeO_3. This crystal exhibits a skyrmion lattice phase near the Curie temperature [1] and a second skyrmion phase at low temperatures [2]. In addition, it has recently been shown that a heterostructure of this chiral magnet with a ferromagnet exhibits hybrid modes in its ferromagnetic resonance spectra [3]. We study magnetization dynamics in a Cu_2OSeO_3 crystal placed in a custom-designed loop-gap microwave cavity and compare the coupling of cavity photons to magnons in Cu_2OSeO_3 to the corresponding coupling between magnons in a $Y_3Fe_5O_{12}$ sphere and the same cavity.

[1] A. Aqeel *et. al*, Phys. Rev. B **103**, L100410 (2021)
[2] A. Chacon *et. al*, Nature Phys **14**, 936-941 (2018)
[3] C. Lüthi *et. al*, Appl. Phys. Lett. **122**, 012401 (2023)

MA 46.17 Thu 15:00 Poster C

Coherent X-ray imaging of Nanoscale spin textures in Ferrimagnetic Multilayers — Tamer Karaman[1], •Manas R. Patra[1,2], Timo Schmidt[1], Riccardo Battistelli[1,2], Christopher Klose[3], Bastian Pfau[3], Manfred Albrecht[1], and Felix Büttner[1,2] — [1]University of Augsburg, 86159 Augsburg, Germany — [2]Helmholtz-Zentrum Berlin, 14109 Berlin, Germany — [3]Max Born Institute, 12489 Berlin, Germany

Chiral rare-earth transition metal ferrimagnets, combining ferromagnetic and antiferromagnetic traits, offer various advantages, including bulk Néel-type Dzyaloshinskii-Moriya interaction (DMI), adjustable anisotropy, and minimal stray fields [1]. Achieving small and yet rapidly moving information-carrying topological spin textures is essential for in-memory and neuromorphic computing technologies [2,3]. This promises to realize high DMI in a thick, compensated material at room temperature. Here we present a coherent x-ray imaging study on Pt/Co/Dy multilayers, which reveals magnetic skyrmions of significant variations in both the size and contrast. While pinning explains size differences, variations in contrast suggest exciting possibilities, such as a 3D spin texture due to a vertical gradient of magnetic properties induced by Dy diffusion or the presence of sub-10-nm-diameter DMI-stabilized skyrmions. This high-resolution imaging holds the promise of uncovering novel physics in the field of nano-magnetism. References: 1. Büttner, F., et al., Sci. Rep. 8, 4464 (2018). 2. Caretta, L. et al., Nat. Nanotechnol. 13, 1154 (2018). 3. Fert, A., et al., Nat. Rev. Mater. 2, 17031 (2017).

MA 46.18 Thu 15:00 Poster C

Mössbauer spectroscopy on $CeFeSb_3$ — •Felix Seewald[1], Manuel Schulze[2], Thomas Doert[2], Michael Ruck[2], and Hans-Henning Klauss[1] — [1]Institut für Festkörper und Materialphysik, TU Dresden, Germany — [2]Fakultät für Chemie und Lebensmittelchemie, TU Dresden, Germany

Rare earth transition metal antimony systems exhibit a wide range of interesting magnetic properties. For example, in $R_3Fe_3Sb_7$ (R = Pr, Nd) we find a complex magnetic structure with R-Fe interplay[1].

The $CeFeSb_3$ structure consists of layers of iron centered $FeSb_2$ octahdera alternating with a Sb square lattice in between Ce layers. The Mössbauer spectrum at room temperature shows a single iron site exhibiting quadrupole splitting due to the presence of an electric field gradient (EFG). The center shift at room temperature is 0.469(3) mms^{-1} relative to α-iron with an EFG principle component of $V_{zz} = \pm 19.1(4)\,VÅ^{-2}$.

Surprisingly even at 4.2 K no static magnetic hyperfine field is detected by Mössbauer, i.e. the spectrum still consists of a single quadrupole split iron site.

We will compare our findings with ferromagnetic order in other transition metal antimony systems.

[1] Falk Pabst, Sabrina Palazzese et. al., Advanced materials

MA 46.19 Thu 15:00 Poster C

Dilatometry studies on van der Waals ferromagnets $Fe_{3-\delta}GeTe_2$, CrI_3 and $Cr_2Ge_2Te_6$ — •Erik Walendy[1], Sven Sprachmann[1], Eva Brücher[2], Rheinhard Kremer[2], and Rüdiger Klingeler[1] — [1]Kirchhoff Institute for Physics, Heidelberg University, Germany — [2]Max Planck Institute for Solid State Research, Stuttgart, Germany

The van der Waals materials $Fe_{3-\delta}GeTe_2$, $Cr_2Ge_2Te_6$ and CrI_3 develop long-range ferromagnetic order down to the monolayer. In the bulk, long-range magnetic order appears at about 220 K, 65 K and 61 K respectively. Our high-resolution capacitance dilatometry studies imply significant magneto-elastic coupling as demonstrated by pronounced anomalies in thermal expansion and magnetostriction. We determine the uniaxial pressure dependencies of T_C and of the dominant energy scales by means of Grüneisen scaling. In $Cr_2Ge_2Te_6$, the magnetic phase diagram is determined and extremely large uniaxial pressure dependencies are observed. In CrI_3, in addition to the

response of the ferromagnetic bulk phase, we find magnetostrictive signatures of the antiferromagnetic surface phase. The comparison of the three materials provides further insight into the relevance of spin-orbit coupling for the development of long-range magnetic order in quasi-2D van der Waals materials.

MA 46.20 Thu 15:00 Poster C

Multi-Q state emerging from frustrated interlayer exchange interaction — •Bjarne Beyer, Mara Gutzeit, Moritz A. Goerzen, and Stefan Heinze — Institute of Theoretical Physics and Astrophysics, University of Kiel, Germany

Superpositions of spin spirals, so-called multi-Q states, are complex spin structures which are of fundamental interest and promising for future spintronic applications. A prominent example is the triple-Q state predicted more than 20 years ago [1] and recently observed in ultrathin Mn films on surfaces [2,3]. Superposition states are energetically degenerate with the corresponding single-Q (spin spiral) states within the Heisenberg model, however, higher-order exchange interactions can lift this degeneracy [1]. Here we propose a three-dimensional multi-Q state in a Mn bilayer that is stabilised by frustrated interlayer exchange interactions. Our study combines ab initio calculations via density functional theory, atomistic spin simulations as well as Fourier analysis and simulation of spin-polarized scanning tunneling microscopy images.

[1] P. Kurz *et al.*, PRL **86**, 1106 (2001).
[2] J. Spethmann *et al.*, PRL **124**, 227203 (2020).
[3] F. Nickel *et al.*, PRB (in press) and arxiv:2307.09764 (2023).

MA 46.21 Thu 15:00 Poster C

The phenomenological model calculations for ultrafast magnetization dynamics — •Jav Davaasambuu, Tsednee Tsogbayar, and Odsuren Sarnai — Institute of Physics and Technology, MAS, Ulaanbaatar, Mongolia

We study ultrafast magnetization dynamics induced by laser heating using various phenomenological temperature models. In this work we have studied the two- and three-temperature models for nickel, iron and cobalt thin films. The temperature dynamics of the electrons, spins and lattice for thin films is investigated. From the 3TM calculation the magnetization dynamics of samples has been obtained as a function of spin temperature, while it is computed using the electron temperature in the 2TM calculation. It has been shown that demagnetization from the 3TM calculation can be clearly related to the increase of the spin temperature. For nickel, we have shown that our numerical result for magnetization is in good agreement with an experimental measurement.

MA 46.22 Thu 15:00 Poster C

Strain engineering of ferroic properties in $AFeO_3$ (A = La, Bi) films — •Antonia Rieche, Aurora Diana Rata, Wolfgang Hoppe, and Kathrin Dörr — Martin-Luther-Universität Halle-Wittenberg

Ferroic properties such as magnetization (M), antiferromagnetic order (L) and ferroelectric polarization (P) can be studied and potentially manipulated with light. An essential prerequisite for this is a successful control of the ferroic domain structures, so that a large mean value of M (L, P) can be achieved. Antiferromagnetic ferrites $AFeO_3$ with weak canted ferromagnetism have shown intriguing optical properties in bulk single crystal, while work on thin films is quite limited due to nanoscopic multidomain coexistence. Here we present results of our attempt to optimize $BiFeO_3$ and $LaFeO_3$ layers for optical experiments. The epitaxial strain controlled by the choice of substrate is used to achieve the formation of structural domains in these ferrite layers in a desirable way. Defined structural domain patterns allow selected orientations and sizes of M, L and P. The films are grown using pulsed laser deposition (KrF 248 nm) and characterized by x-ray diffraction, magnetooptical Kerr effect and scanning probe microscopies.

MA 46.23 Thu 15:00 Poster C

A theoretical study of new polar and magnetic double perovskites for photovoltaic applications — •Neda Rahmani[1], Alireza Shabani[2], and Jost Adam[3] — [1]Niels Bohr International Academy, Niels Bohr Institute, University of Copenhagen, Copenhagen, Denmark — [2]Department of Electrical and Photonics Engineering, Photonic Nanotechnology, NanoPhoton, Technical University of Denmark (DTU), Copenhagen, Denmark — [3]Computational Materials and Photonics, Kassel University, Kassel, Germany

Searching for novel functional materials has attracted significant interest for the breakthrough in photovoltaics to tackle the prevalent energy crisis. Through density functional theory calculations, we evaluate the structural, electronic, magnetic, and optical properties of new double perovskites Sn2MnTaO6 and Sn2FeTaO6 for potential photovoltaic applications. Our structural optimizations reveal a non-centrosymmetric distorted triclinic structure for the compounds. Using total energy calculations, antiferromagnetic and ferromagnetic orderings are predicted as the magnetic ground states for Sn2MnTaO6 and Sn2FeTaO6, respectively. The empty d orbitals of Ta5+-3d0 and partially filled d orbitals of Mn/Fe are the origins of ferroelectricity and magnetism in these double perovskites resulting in the potential multiferroicity. The structural stability, suitable band gap, and high absorption coefficient values of proposed compounds suggest they could be good candidates for photovoltaic applications.

MA 46.24 Thu 15:00 Poster C

Electrically controlled magnetoeletric switching in a multiferroic — Sergey Artyukhin[2], Louis Ponet[2], Janek Wettstein[1], Alexey Shuvaev[1], Maxim Mostovoy[3], Andrei Pimenov[1], Anna Pimenov[1], and •Maksim Ryzhkov[1] — [1]Institute of Solid State Physics, Vienna University of Technology, Vienna, Austria — [2]Quantum Materials Theory, Istituto Italiano di Tecnologia, Genova, Italy — [3]Zernike Institute for Advanced Materials, University of Groningen, Groningen, The Netherlands

Electric control of magnetism and magnetic control of ferroelectricity can improve the energy efficiency of magnetic memory and data-processing devices. However, the necessary magnetoelectric switching is hard to achieve, and requires more than just a coupling between the spin and the charge degrees of freedom. Recently, we showed that an application and subsequent removal of a magnetic field reverses the electric polarization of the multiferroic $GdMn_2O_5$, thus requiring two cycles to bring the system back to the original configuration. During this unusual hysteresis loop, four states with different magnetic configurations are visited by the system, with one half of all spins undergoing unidirectional full-circle rotation in increments of about 90 degrees. Our findings established a paradigm of topologically protected switching phenomena in ferroic materials.

Here I will present further study on electrically controlled magnetoelectric switching in the multiferroic $GdMn_2O_5$. We show that the sign of the resulting polarization can be precisely manipulated based on the direction of the electric field.

MA 46.25 Thu 15:00 Poster C

Sprayed nanometer-thick hard magnetic coatings with strong perpendicular anisotropy for data-storage applications — •A. Chumakov[1], C.J. Brett[1,2], K. Gordeyeva[2], D. Menzel[3], L.O.O. Akinsinde[4,5], M. Gensch[1], M. Schwartzkopf[1], W. Cao[6], S. Yin[6], M.A. Reus[6], M.A. Rübhausen[4], P. Müller-Buschbaum[6], L.D. Söderberg[2], and S.V. Roth[1,2] — [1]DESY, Hamburg, Germany — [2]KTH, Stockholm, Sweden — [3]Technische Universität Braunschweig, Braunschweig, Germany — [4]Universität Hamburg, Hamburg, Germany — [5]Kiel University, Kiel, Germany — [6]Technische Universität München, Garching, Germany

Ferromagnetic $SrFe_{12}O_{19}$ nanoparticles with a solid magnetic moment perpendicular to their plane and stabilized by a positive surface charge can form a self-ordered coating under the influence of magnetic fields drying from dispersion. We investigated the film formation of a stable colloid dispersion of ferromagnetic nanoplates and nanoblocks onto a silicon substrate and cellulose nanofilm without and under the action of an external magnetic field during scalable layer-by-layer spraying. The formation of a film of ferromagnetic particles from an aqueous colloid makes it possible to form a stable magnetic coating of agglomerates of nanoparticles with a fractal structure. An external magnetic field in the deposition process leads to the appearance of residual magnetization in the film. In this case, particles with a smaller aspect ratio (nanoblocks) form a periodic structure of agglomerates of nanoparticles with signs of an artificial opal-like structure.

MA 46.26 Thu 15:00 Poster C

Studying the electronic band structure of the exfoliated two-dimensional antiferromagnet $NiPS_3$ via temperature dependent μ-ARPES — Benjamin Pestka[1], •Biplab Bhattacharyya[1], Jeff Strasdas[1], Miłosz Rybak[2], Adi Harchol[3], Niklas Leuth[1], Honey Boban[4], Vitaliy Feyer[4], Iulia Cojocariu[4], Daniel Baranowski[4], Simone Mearini[4], Lutz Waldecker[1], Bernd

Beschoten[1], Christoph Stampfer[1], Marcus Liebmann[1], Lukasz Plucinski[4], Efrat Lifshitz[3], Magdalena Birowska[5], and Markus Morgenstern[1] — [1]RWTH-Aachen University, Germany — [2]Wrocław University of Science and Technology, Poland — [3]Technion - Israel Institute of Technology, Haifa, Israel — [4]Forschungszentrum Jülich, PGI-6, Germany — [5]University of Warsaw, Poland

Two-dimensional (2D) anti-ferromagnetic (AFM) materials offer novel research directions due to the pronounced interaction of electronic, spin and lattice structure. Transition metal phosphorus trisulfides ($TMPS_3$) are a semiconducting class of 2D AFM materials with intralayer AFM order. Till date, the role of the electronic band structure for AFM coupling in exfoliated thin flakes of $TMPS_3$ has often remained unexplored. Here, we present a comprehensive study of temperature dependent angle-resolved photoemission spectroscopy (ARPES) of the exfoliated few-layered $NiPS_3$ above and below the Néel temperature (T_N). We observe band spectra changes across T_N that are compared with density functional theory data to pinpoint their orbital character. The AFM transition in our exfoliated flakes has been verified by Raman spectroscopy.

MA 46.27 Thu 15:00 Poster C

Surface roughness optimization of 2D and 3D 2-Photon Polymerization Lithography templates and their influence on magnetic thin film properties — •Christian Janzen, Bhavadip Bharatbhai Rakholiya, Florian Ott, Rico Huhnstock, and Arno Ehresmann — Institute of Physics and Center for Interdisciplinary Nanostructure Science and Technology (CINSaT), University of Kassel, Kassel, Germany

To experimentally investigate the impact of geometry and curvature on the properties of magnetic thin film systems, micron-sized slanted/curved structures were prepared by 2-photon polymerization (2PP) lithography. By systematically varying the 2PP process parameters, the root-mean-square roughness of 2D/3D shaped structures is minimized. Adding a Cu buffer layer, further smoothening of the surface was achieved, as atomic force microscopy measurements show. Elevating the structures with lithographically produced spacers allows us to investigate two scenarios for the deposition of a magnetic thin film on top of these structures: (1) the 2D/3D magnetic film is connected to surrounding flat film (no spacer) and (2) the 2D/3D magnetic film is isolated (with spacer). Therefore, it is possible to tune the exchange and dipolar interaction of 2D/3D microstructured magnetic thin films. The magnetic properties of a ferromagnetic thin film as a function of the surface roughness and shape anisotropy (i.e., the geometry of the templating structure) are investigated using magneto-optical Kerr microscopy.

MA 46.28 Thu 15:00 Poster C

Electron-phonon interaction, magnetic phase transition, charge density waves and resistive switching in VS2 and VSe2 revealed by Yanson PCS — Dmytro Bashlakov[1], •Oksana Kvitnitskaya[2,1], Saicharan Aswartham[2], Luminita Harnagea[3], Dmitri Efremov[2], Bernd Büchner[2,4], and Yuri Naidyuk[1] — [1]B. Verkin Institute for Low Temperature Physics & Engineering, NASU, Kharkiv, Ukraine — [2]Leibniz-Institute for Solid State Research, IFW Dresden, Dresden, Germany — [3]Dep. of Physics, Indian Institute of Science Education and Research, Pune, India — [4]Institute of Solid State and Materials Physics and Würzburg-Dresden Cluster of Excellence ct.qmat, TU Dresden, Dresden, Germany

The transition metals dichalcogenides VS2 and VSe2 possess promising properties as to magnetic and CDW ordering, emergent superconductivity, which are very sensitive to the stoichiometry and dimensionality. Yanson point-contact (PC) spectroscopic study reveals metallic and nonmetallic state in VS2 PCs, as well as magnetic phase transition below 25 K. PC spectra of VS2 testifies to the thermal regime, although the rare PC spectrum has a broad maximum at 20 mV due to electron-phonon interaction (EPI). PC spectra of VSe2 show metallic behavior with the features associated to EPI and CDW. The Kondo effect, which appeared for both compounds, is apparently due to interlayer V-ions. A resistive switching between a low-resistance metallic state and a high-resistance non-metallic state was observed in the PC on VSe2. The alteration of stoichiometry in PC core due to displacement of V-ions to interlayer under high electric field may be the reason.

MA 46.29 Thu 15:00 Poster C

Skyrmion dynamics in confined structures — •Thomas Brian Winkler[1], Jan Rothörl[1], Maarten Brems[1], Grischa Beneke[1], Hans Fangohr[2], and Mathias Kläui[1] — [1]Institute of Physics, Johannes Gutenberg University, Staudinger Weg 7, 55128 Mainz, Germany — [2]Max Planck Institute for the Structure and Dynamics of Matter Hamburg, Luruper Chaussee 149, 22761 Hamburg

Magnetic skyrmions are fascinating spin structures from a physics perspective due to their topological stabilization but are also considered for next-generation non-conventional computing devices [1,2]. Skyrmions must be hosted in a finite-sized sample for a device application, and the dynamics can differ from those in continuous film geometries. We investigate the dynamics of a driven confined skyrmion ensemble and find different meta-stable states to occur [3].

[1] K. Everschor-Sitte et al., Journal of Applied Physics 124, 240901 (2018). [2] K. Raab et al., Nat Commun 13, 6982 (2022) [3] Thomas Brian Winkler et al., arxiv:2303.16472 (2023)

MA 46.30 Thu 15:00 Poster C

Characterizing the defocusing behaviour of magnetic microparticles for the application in three-dimensional trajectory tracking — •Nikolai Weidt, Yahya Shubbak, Rico Huhnstock, and Arno Ehresmann — Department of Physics and Center for Interdisciplinary Nanostructure Science and Technology (CINSaT), University of Kassel, Heinrich-Plett-Str. 40, D-34132 Kassel

To realise Lab-on-a-chip systems superparamagnetic particles (SPPs) can be surface-functionalized to bind specific analytes [1]. The directed transport of SPPs above magnetically stripe-patterned exchange bias layer systems is a promising approach to achieving analyte binding and transfer [2]. Precise analysis of three-dimensional SPP trajectories in this system can lead to the detection of analyte-binding events. To access the third dimension, the defocusing of particles moving out of the microscope's focal plane during transport steps is measured [3]. In this work, the quantization of defocusing is done by determining the Tenenbaum gradient (TG) of single particles. Using a calibration procedure, the z-coordinate of SPPs is derived from the measured TG. The obtained 3D trajectories are confirmed by numerical simulations for SPP motion. [1] Rampini, S., Li, P., Lee, G.U., 2016. Lab on a Chip 16, 3645*3663. [2] D. Holzinger, I. Koch, S. Burgard, and A.Ehresmann, ACS Nano 9, 7323 (2015) [3] Huhnstock, R., Reginka, M., Sonntag, C., Merkel, M., Dingel, K., Sick, B., Vogel, M., Ehresmann, A., Sci Rep 12, 20890.

MA 46.31 Thu 15:00 Poster C

Structural and magnetic characterization of FeOx nanoparticle dispersions upon freezing and melting — •Maximilian Enneking[1,2], Asmaa Qdemat[1], Martin Dulle[3], Rolf J. Haug[4], and Oleg Petracic[1,5] — [1]Jülich Centre for Neutron Science JCNS-2 und Peter Grünberg Institut PGI-4, Forschungszentrum Jülich GmbH — [2]Faculty of Mathematics and Physics, Leibniz Universität Hannover — [3]Jülich Centre for Neutron Science (JCNS-1), Forschungszentrum Jülich GmbH — [4]Institute of Solid State Physics, Leibniz Universität Hannover — [5]Heinrich Heine University Düsseldorf, Faculty of Mathematics and Natural Sciences, Düsseldorf

We have studied the structural and magnetic properties of magnetic nanoparticle dispersions upon cooling and heating over the solvent melting temperature. The particles consist of iron oxide dispersed in water or toluene with diameters ranging from 10 to 20 nm. The magnetic properties were studied using SQUID magnetometry employing zero field cooled (ZFC)/field cooled (FC) magnetization curves at different fields and hysteresis curves. To investigate the influence of temperature on the properties of nanoparticles and their assemblies, in situ SAXS measurements were performed at variable temperatures. We observe distinct freezing/melting signatures in magnetometry of the nanoparticle-solvent system depending on the particle size and the type of solvent.

MA 46.32 Thu 15:00 Poster C

Towards Recycling of Nd-Fe-B Permanent Magnets in a Circular Economy — •Aybike Paksoy[1], Amrita Khan[1], Abdullatif Durgun[1], Mario Schönfeldt[2], Hasan Mahmudul[2], Iliya Radulov[2], Imants Dirba[1], and Oliver Gutfleisch[1] — [1]TU Darmstadt, Department of Materials and Geosciences, Functional Materials, Germany — [2]Fraunhofer IWKS, Fraunhofer Research Institution for Materials Recycling and Resource Strategies, Germany

Nd-Fe-B magnets have the highest room temperature energy product (BH)max and therefore are the material of choice in various application areas critical to the clean energy transition. However, usage of critical rare earth elements creates a number of environmental, economic as well as geopolitical concerns related to China which is the main global

exporter. Exhaust gas and waste water are generated in significant amounts by the chemicals needed for the rare earth mining and refining processes. If not handled properly, it will have a huge impact on the environment, causing groundwater pollution and geological deterioration. This pollution affects humans as well in the circular ecosystem, and subsequent environmental governance comes at a heavy cost. Therefore, companies and researchers have been gradually focusing on the recycling of back-end waste Nd-Fe-B permanent magnets. For an environmentally friendly product, it is necessary to reduce the criticality and increase the sustainability of rare earth permanent magnets. In this study, we investigate advanced recycling processing towards sustainable Nd-Fe-B magnets without sacrificing the performance.

MA 46.33 Thu 15:00 Poster C

Effect of Zr and Cu alloying elements on microstructure and magnetic properties of Sm2Co17-type magnets — •B. Ekitli[1], A. Aubert[1], F. Maccari[1], N. Polin[2], X. Chen[2], E. Adabifiroozjaei[3], L. Molina-Luna[3], B. Gault[2], K. Skokov[1], and O. Gutfleisch[1] — [1]FM, TU Darmstadt, Germany — [2]MPIE, Düsseldorf, Germany — [3]AEM, TU Darmstadt, Germany

Hard magnetic properties of 2:17-type Sm(CobalFewCuyZrx)z magnets are mainly controlled by domain wall pinning. The complex microstructure including a superposition of 2:17 cells, 1:5 cell boundaries, and Zr-rich z-lamellae is essential for optimal performance [1]. In addition, the microchemistry is key for pinning through Cu gradient concentration and layers in the 1:5 cell boundaries [2]. Within this complex composition and microstructure, each element plays a distinct role in developing the desired phases and magnetic properties. In this study, we focus on studying the influence of Cu and Zr content in developing the microstructure and hard magnetic properties using simpler composition than commercial ones. A systematic study has been conducted using the Sm(CobalCuyZrx)z composition, excluding Fe, with the values x= 0.023 & 0.031, y= 0-0.30, and z= 6.7 & 7.7. Thus, we can reveal the individual role of Zr and Cu for optimum magnetic performance through detail analysis of the magnetic properties (hysteresis and domain structure observation) and correlate them with microstructure (SEM, TEM and APT). We acknowledge funding by CRC TRR 270 HoMMage. [1] Gutfleisch, O. (2009). DOI: 10.1007/978-0-387-85600-1_12 [2] S. Giron et al (2024)

MA 46.34 Thu 15:00 Poster C

Two-powder method for heavy rare earth reduced sintered NdFeB magnets — •Abdullatif Durgun[1], Konrad Opelt[2], Chi-Chia Lin[2], Jürgen Gassmann[2], Imants Dirba[1], and Oliver Gutfleisch[1] — [1]TU Darmstadt, Department of Materials and Geosciences, Functional Materials, 64287 Darmstadt, Germany — [2]Fraunhofer IWKS, 63457 Hanau, Germany

Nd2Fe14B magnets play crucial role in e-motor technology, enhancing efficiency and power density. However, their use in high-temperature motors (up to 200 °C) is limited due to the low Curie temperature and decreased coercivity. As a result, NdFeB magnets require high coercivity (*2400 kA/m) at room temperature for effective operation in high-temperature e-motor applications. This can be achieved by replacing Nd atoms with heavy rare earths like Dy or Tb, however with significantly increased costs and reduced magnetization. Therefore, this study aims to improve the thermal stability and coercivity of sintered NdFeB magnets by forming (Nd,Dy/Tb)2Fe14B-rich shells around the Nd2Fe14B grains. Sintered NdFeB magnets were fabricated via our patented 2-powder-method [1,2] using NdFeB main phase and Dy/Tb-rich high-anisotropy powders. The impact of powder particle size, alloy composition and mixing ratios is systematically investigated to optimize the magnet microstructure and magnetic properties. Forming (Nd,Dy/Tb)2Fe14B shells around the NdFeB core boosts coercivity without significant magnetization loss, enabling the use of cost-and-resource-efficient and large volume NdFeB magnets at high temperatures.

MA 46.35 Thu 15:00 Poster C

Homogeneous permanent magnetic field for magnonic applications — •Gabriel Schwöbel, Vitaliy I. Vasyuchka, Aleksander A. Serga, and Burkard Hillebrands — Fachbereich Physik and Landesforschungszentrum OPTIMAS, Rheinland-Pfälzische Universität Kaiserslautern Landau, 67663 Kaiserslautern, Germany

Our work addresses the development of a homogeneous permanent magnetic field experimental setup for a variety of applications, primarily in the field of magnonics. Particularly sensitive are spin-wave phase measurements, which require a high degree of homogeneity, as well as the minimisation of any noise that might be imposed by using an electromagnet.

The setup is inspired from a paper which includes two NeFeB permanent magnets, a soft magnetic yoke and pole shoes. The main goal is to figure out a suitable shape of the yoke and the pole shoes which provide a homogenious magnetic flux distribution over macroscopic distances (e.g. 10 mm) with. To achieve this goal, COMSOL Multiphysics was used to simulate the field strength distribution for different shapes of pole shoes.

We analysed different types of pole shoes to ensure improved homogeneity for different gap sizes. Since the required homogenity is approximately given by the line width of the spin wave excitations studied in yttrium-iron garnet, we looked for a value of around 50 μT in a 1 cm cube centred on the gap.

MA 46.36 Thu 15:00 Poster C

Insights into the electronic structure of Ce-substituted permanent magnets — •Benedikt Eggert[1], Alex Aubert[2], Fabrice Wilhelm[3], Andrei Rogalev[3], Konstantin Skokov[2], Heiko Wende[1], Oliver Gutfleisch[2], and Katharina Ollefs[1] — [1]Faculty of Physics and CENIDE, University of Duisburg-Essen — [2]Functional Materials, Technical University of Darmstadt — [3]European Synchrotron Radiation Facility

Permanent magnets significantly contribute to renewable energy technologies based on their broad range of potential applications [1]. The relatively low abundance of rare-earth elements such as Nd and Sm motivates additional research into cost-effective hard magnetic materials by replacing Nd or Sm with more abundant rare-earth materials, such as Ce, Pr or La. With this contribution, we investigate the magnetic properties of Ce-substituted Nd-Fe-B [2] or Ce-Co permanent magnets utilizing X-ray absorption spectroscopy and X-ray magnetic circular dichroism. We will correlate how the system's magnetic properties depend on Ce's valence state.

We acknowledge the financial support through the Deutsche Forschungsgemeinschaft within the framework of the CRC/TRR270 HoMMage (Project 405553726-TRR270), the BMBF (05K2019 and 05K2022), and we thank the ESRF for allocation of beamtime at the beamline ID12 within project HC-4051.

[1] O. Gutfleisch et al. Adv. Mater. 23, 821-842 (2011)
[2] Y. Wu et al. Acta Materialia, 235, 118062 (2022)

MA 46.37 Thu 15:00 Poster C

Magnetic Interaction in the Frustrated Dimer Magnet $Cs_3Fe_2Br_9$ — •Felix Wirth[1], Sebastian Biesenkamp[1], Alexandre Bertin[1], Dimitry Gorkov[1], Ivan Sidis[2], Jakob Lass[3], Rafal Wawrzynczak[3], Petra Becker-Bohatý[4], Ladislav Bohatý[4], and Markus Braden[1] — [1]II. Physic. Inst., Univ. Cologne, Germany — [2]LLB, CEA Saclay, France — [3]SINQ, PSI Villigen, Switzerland — [4]Inst. Geology a. Mineralogie, Univ. Cologne, Germany

The frustrated magnet $Cs_3Fe_2Br_9$ with Fe_2Br_9 bioctahedron dimers in a triangular lattice exhibits a remarkable variety of magnetic phases, when magnetic fields are applied along the c-axis and huge magnetoeleastic anomalies [1]. In addition, there are magnetization plateaus for H||c, while magnetization for H||a,b stays linear up to saturation [1]. Here we present additional neutron scattering experiments to further elucidate the character of magnetic correlations. While at low temperature and zero field, magnetic order is commensurate with parallel moments in a dimer, a competing phase is incommensurate. Inelastic neutron scattering studies on the multiplexing spectrometer CAMEA determined the dispersion of magnons in the ordered phase over a wide range of Q space. The results were analyzed by linear spin-wave calculations with *SpinW* yielding a rather 3D character of the magnetism. However, low-energy magnon response in the ordered state as well as the diffuse and quasielastic scattering in the intermediate and paramagnetic phases are smeared over large parts on the Brillouin zone boundary, further characterizing this system as a peculiar frustrated magnet. [1] D. Brüning, et al. Phys. Rev. B. 104 (2021).

MA 46.38 Thu 15:00 Poster C

Indications of dynamical magnetism in magnetically ordered Kagome metals
— •Sheetal Devi[1], Yishui Zhou[1], Min-Kai Lee[2], Lieh-Jeng Chang[2], Hubertus Luetkens[3], Zurab Guguchia[3], and Yixi Su[1] — [1]Jülich Centre for Neutron Science JCNS at Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH, Lichtenbergstraße 1, D-85747 Garching, Germany

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— [3]Laboratory for Muon Spin Spectroscopy, Paul Scherrer Institute, CH-5232, Villigen PSI, Switzerland

We have investigated the low-temperature physical properties of topological intermetallic compounds RV_6Sn_6 (R = Tb, Dy, Ho, Er) using heat-capacity and muon spin relaxation (μSR) measurements. These compounds feature a combination of a V-based nonmagnetic Kagome sublattice and an R-based magnetic triangular sublattice that harbors different spin anisotropies for different R ions. Long-range magnetic order is seen for R = Tb, Dy, Ho, and Er compounds at 4.3, 3.0, 2.4, and 0.6 K, respectively. However, the hyperfine analysis of the heat capacity data yields a reduced value of magnetic moment for all the compounds, implying persistence spin fluctuations down to 50 mK. Indications of such dynamical magnetism are further supported by our μSR studies. We argue that this intriguing competition and coexistence between persistent spin dynamics and long-range magnetic order is a manifestation of strong magnetic frustration in these systems.

MA 46.39 Thu 15:00 Poster C

Single-crystal-diffraction studies on the iron-superconductor parent compounds LaFeAsO and SmFeAsO — •Akshay Tewari[1], Felix Anger[2], Alexandre Bertin[1], Bernd Büchner[2], Sabine Wurmehl[2], and Markus Braden[1] — [1]II. Phys. Inst., Univ. Cologne, Germany — [2]IFW, Dresden, Germany

Iron-based superconductors exhibit a complex interplay between structure, magnetism and superconductivity. Here, we report detailed X-ray diffraction single-crystal structure analyses on the *1111* family of FeAs superconductors REFeAsO, where RE is La or Sm. Previous powder neutron diffraction measurements on LaFeAsO revealed tiny structural anomalies occurring around the structural and magnetic transitions.

The crystal structure is tetragonal at room temperature, and a structural transition occurs at 160-170 K into the orthorhombic phase. In the tetragonal phase we observe reflections violating the h+k=2n condition at low (hk0) values. These peaks are attributed to multiple diffraction arising from the high crystal quality. Below the structural transition, the appearance of orthorhombic domains reduces the crystal quality and thus multiple diffraction. We find no evidence for additional scattering centers (or residual electron density) in the unit cell. Structural anomalies observed for the Fe-As distance and FeAs layer thickness around the transition temperature tend to agree with previous measurements performed using powder data [1]. Anharmonic refinements (up to 4th order) indicate non-harmonic distributions appearing around the La and As atoms near the transition temperatures.

MA 46.40 Thu 15:00 Poster C

Thermodynamic properties of the checkerboard model of altermagnet — •Kostiantyn Yershov[1,2], Volodymyr Kravchuk[1,2], and Jeroen van den Brink[1] — [1]Leibniz Institute for Solid State and Materials Research, Dresden, Germany — [2]Bogolyubov Institute for Theoretical Physics, Kyiv, Ukraine

Using the checkerboard Hubbard hamiltonian as a model for two-dimensional altermagnet, we demonstrated that the temperature-induced fluctuations can lead to several new effects, namely the fluctuation induced piezomagnetism and thermal spin conductivity. First, computing the dispersion relation for magnons, we demonstrated that the model under consideration breaks the spin degeneracy in the momentum space leading to the anisotropic splitting of magnon branches typical for the altermagnets. Next, in the limit of low temperatures we considered the thermally induced magnons as an ideal Bose gas and computed the thermodynamic potential accordingly. Using the thermodynamic potential, we computed magnetization M as a thermodynamic quantity, and demonstrated that M vanishes for vanishing magnetic field. However, M is finite beyond the altermagnetic limit, when the diagonal terms in the checkerboard model becomes not equivalent, e.g. due to the applied mechanical stress. In addition, we predict generation of the spin-current in the response to the applied temperature gradients. We calculated the tensor of thermal spin conductivity, which is linear with diagonal terms of checkerboard model for small temperatures.

MA 46.41 Thu 15:00 Poster C

Magnetism in ultrathin quantum spin liquid Na_2IrO_3 flakes — •Deepak Roy and Mukul Kabir — Department of Physics, IISER Pune - 411008, India

Quantum spin liquids have attracted significant attention due to their complex physics arising from the interplay among the lattice geometry, spin-orbit coupling, and electron correlation. The Ir^{4+} oxides and Ru^{3+} chlorides possessing a honeycomb $j_{\text{eff}} = 1/2$ lattice are the primary candidate materials, which eventually exhibit long-range ordering at low temperatures. Using first-principles calculations, we explore ultrathin Na_2IrO_3 flakes to find that the zigzag antiferromagnetic ground state persists up to the monolayer. Magnetic ordering is investigated using appropriate Kitaev-Heisenberg Monte Carlo simulations. Surprisingly, the magnetic state is reinforced, and the monolayer is driven away from the Kitaev spin liquid state due to stronger Heisenberg and off-diagonal exchange interactions. In contrast, the charge-doped flakes undergo a Mott insulator-to-metal transition, and the flakes become ferromagnetic. These results illustrate exciting prospects for understanding magnetism in ultrathin non-van der Waals correlated oxides and their prospect in spin devices.

MA 46.42 Thu 15:00 Poster C

Magnetic phase diagram of Kitaev Quantum Spin Liquid candidate $Na_3Co_2SbO_6$ — •Kranthi Kumar Bestha[1,2], Manaswini Sahoo[1,2], Ryan Christopher Morrow[1], Andrey Maljuk[1], Bernd Büchner[1,2], Laura Teresa Corredor Bohorquez[1], and Anja U. B. Wolter[1] — [1]Institute for Solid State Research, Leibniz IFW Dresden 01069, Dresden, Germany — [2]Institute of Solid State and Materials Physics, TU Dresden, 01062 Dresden, Germany

The quest for exotic Quantum Spin Liquids (QSL) with the most entangled quantum states, particularly in Kitaev Quantum Spin Liquid candidates, has posed significant challenges in the last two decades. The presence of non-Kitaev interactions has been a primary obstacle, as they destabilize the QSL ground state. To overcome this hurdle, a search for candidates with more localized d-orbitals, such as $3d$ cobaltates, was proposed, aiming to eliminate non-Kitaev interactions despite their weak spin-orbit interaction. In this study, we employed thermodynamic methods to characterize such a cobaltate KQSL candidate, $Na_3Co_2SbO_6$ (NCSO). Our investigations, including *M(H,T)* and $C_p(T)$ studies on high quality single crystals, confirm AFM order in NCSO at $T_N = 7$ K. Our *M(T)* data reveal that NCSO is an easy-plane magnet with large anisotropy in *ab*-plane and two metamagnetic transitions, manifestation of field-induced phases in the ordered phase. From the *M(H)*, *M(T)* and $C_p(T)$ data we mapped out the magnetic phase diagram of NCSO in the light of theoretical predictions.

MA 46.43 Thu 15:00 Poster C

Field induce transition and quantum criticality in spin-$\frac{3}{2}$ stacked-honeycomb antiferromagnet: $Ba_2Co(PO_4)_2$ — •Aditi Agrawal[1], Koushik Chakraborty[1], Isha Isha[1], K. M. Ranjith[2], M. Baenitz[2], M. Isobe[3], A. K. Bera[4], and Arvind Kumar Yogi[1] — [1]UGC-DAE Consortium for Scientific Research, University Campus, Khandwa Road, Indore 452001, India — [2]Khandwa Road — [3]Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, D-70569 Stuttgart, Germany — [4]Solid State Physics Division, Bhabha Atomic Research Centre, Mumbai 400085, India

We report the bulk and local probe studies on $Ba_2Co(PO_4)_2$ with stacked-honeycomb lattices of cobalt ions on the *bc*-plane. Through a combination of magnetic susceptibility, specific heat, and ^{31}P NMR studies, the temperature-magnetic-field phase diagram associated with this long range magnetic ordering $T_N = 3$ K has been mapped out. A low-temperature field-induced spin-flop transition and spin-reorientation transition below T_N is found to occur at an applied field of $\sim$3 Tesla and $\sim$10 Tesla respectively. The temperature dependent susceptibility curve $\chi(T)$ also shows pronounced broad peak, characteristics of the short-range magnetic ordering, with $T_{max} = 4$ K. The combined results of heat capacity and susceptibility of $Ba_2Co(PO_4)_2$ stabilize a magnetic field induce phase transition. Interestingly, the quantum critical point (QCP) of the phase transition is determined from the extrapolation of the behaviour of T_N as a function of magnetic field on H-T phase diagram. The extrapolated QCP is found at a upper critical field ($H_C \sim 6.5$ T

MA 46.44 Thu 15:00 Poster C

Magnetic properties of the spin-1/2 zigzag chain lattice antiferromagnet: $CaCuV_2O_7$ — •Koushik Chakraborty[1], Aditi Agrawal[1], Isha Isha[1], Suman Karmakar[1], R. Rawat[1], M. Isobe[2], and Arvind Kumar Yogi[1] — [1]UGC-DAE Consortium for Scientific Research, University Campus, Khandwa Road, Indore-452001, India — [2]Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, D-70569 Stuttgart, Germany

We report the magnetic properties of a new CuO_4 plaquette spin-1/2 zigzag chain compound $CaCuV_2O_7$, which ordered antiferromagnetically (AFM) below T_N = 2.4 K, and it reveals the 3*d* characteristics of a nearly divalent Cu^{2+} ion moment obtained from our Curie-Weiss (CW) magnetic susceptibility analysis. The effective magnetic moment μ_{eff} is calculated to be 1.83 (2) μ_B, which is in good agreement with the Cu^{2+} ions for a $S = \frac{1}{2}$ and a g value of 2 (free-electron g-value). The negative Weiss constant θ_{CW} = -18.9 K, as found to be from susceptibility CW fit, suggests that the dominant interactions between Cu^{+2} ions are of AFM. Interestingly, it is also found that the application of the applied magnetic field at H = 9T suppresses the magnetic ordering.

MA 46.45 Thu 15:00 Poster C

Interplay of electronic and lattice-mediated interactions in low-temperature orders of Ba2MgReO6 — •Dario Fiore Mosca[1,2], Cesare Franchini[3,4], and Leonid V. Pourovskii[1,2] — [1]Centre de Physique Theorique, Ecole Polytechnique, Paris, France — [2]College de France, Paris, France — [3]University of Vienna, Vienna, Austria — [4]University of Bologna, Bologna, Italy

The synergetic interaction of electron correlations and strong spin-orbit coupling can lead to the development magnetic and charge orders of high-rank multipoles. In this context, double perovskites with 5d1 electronic configuration offer a opportunity for investigating such phenomena, especially for realizing "hidden" quadrupolar phases.

In our study, we combine several ab-initio techniques that include DFT, DMFT, Jahn-Teller and phonon analysis as well as calculations of intersite exchange interactions using a many-body force-theorem method. This multifaceted approach successfully reproduces the double-step transition observed in Ba2MgReO6; namely, the formation of a higher-temperature anti-ferro quadrupolar phase followed by the onset of a canted anti-ferromagnetic state.

Our analysis reveals that those phases emerge from a complex interplay between the electronic superexchange mechanism and electron-lattice interactions. Additionally, our study clarifies the evolution of the low-temperature order under pressure, in particular, revealing a strong impact of non-hydrostatic pressure condition on the phase stability of Ba2MgReO6.

MA 46.46 Thu 15:00 Poster C

Growth, characterization and neutron scattering studies of $Sr_xCa_{1-x}RuO_3$ ($x = 0.5, 0.7$) single crystals — •Zahrasadat Ghazinezhad[1], Akshay Tewari[1], Karin Schmalzl[2,3], and Markus Braden[1] — [1]II. Physikalisches Institut, Universität zu Köln, Köln, Germany — [2]Jülich Centre for Neutron Science, Jülich, Germany — [3]Institut Laue-Langevin, Grenoble, France

The ferromagnetic order in $SrRuO_3$ attracts strong interest due to the impact of Weyl points on the magneto transport and on the spin dynamics, see [1]. Substituting Sr with isovalent Ca ion reduces the ferromagnetic transition temperature and completely suppresses the ferromagnetism state around 70 percent Ca doping. The smaller Ca ion causes enhanced octahedron tilting, which decreases the FM interaction and seems to imply antiferromagnetic interaction. The comprehensive studies of the spin-wave dispersion in $SrRuO_3$ already indicate some AFM interaction [1]. We grew large single-crystals of $Sr_xCa_{1-x}RuO_3$ ($x = 0.5, 0.7$) by the floating-zone technique. Inelastic neutron scattering studies were performed for both concentrations on the cold triple-axis spectrometer IN12 at the ILL. While $SrRuO_3$ exhibits the expected parabolic dispersion starting at a well defined anisotropy gap, both mixed materials show rather unusual magnetic response in the ordered phase. In spite of the reduced Curie temperatures the anisotropy gap seems to be strongly enhanced and even splits. Furthermore, there is finite scattering at the ferromagnetic zone center even below these gap values.

[1] K. Jenni, et al. , Phys. Rev. B 107, 174429 (2023).

MA 46.47 Thu 15:00 Poster C

Crystal structure and magnetic excitations of Sr4Ru3O10 — Zahrasadat Ghazinezhad[1], •Lara Kiefer[1], Augustinus Agung Nugroho[2], Paul Steffens[3], Ursula Bengaard Hansen[3], and Markus Braden[1] — [1]II. Physic. Inst., Univ. Cologne, Germany — [2]Institut Teknologi Bandung, Indonesia — [3]ILL, Grenoble, France

Large single-crystals of the triple layer ruthenate $Sr_4Ru_3O_{10}$ were grown by the floating zone technique in a mirror image furnace and characterized by X-ray diffraction, magnetization and resistance measurements. Comprehensive single-crystal X-ray diffraction studies reveal that the spacegroup is orthorhombic *Bbcm* and not *Pbam*, mostly used to describe the structure of $Sr_4Ru_3O_{10}$ [1]. RuO_6 octahedra are rotated around the axis perpendicular to the layers, but there is no additional tilting. The onset of ferromagnetic order at 105 K and the low-temperature ordered moment of 1.3 μ_B agree with earlier reports. The magnon dispersion was studied on the triple-axis spectrometers IN20 and Thales at the ILL. We find a parabolic isotropic dispersion with a stiffness constant that is comparable to that observed in the 3D material $SrRuO_3$ [2]. However, the detailed distribution of spin-wave scattering at low constant energy transfer deviates from the simple isotropic ring expected in the most simple model and the stiffness tends to increase upon heating again resembling the behavior in $SrRuO_3$ [2]. The spin-wave gap exhibits a rather anomalous temperature dependency with a strong increase upon cooling below 60 K.

[1] M. K. Crawford *et al.*, Phys. Rev. B **65**, 214412 (2002).
[2] K. Jenni *et al.*, Phys. Rev. Lett. **123**, 017202 (2019).

MA 46.48 Thu 15:00 Poster C

Disentangling the ferrimagnetic moment arrangement in the Ti-doped Barium hexaferrite using EMCD — •Hitoshi Makino[1], Rolf Erni[2], Bernd Rellinghaus[1], and Darius Pohl[1] — [1]DCN, cfaed, TUD Dresden University of Technology, Germany — [2]Empa, Swiss Federal Laboratories for Materials Science and Technology, Dübendolf, Switzerland

Barium hexaferrite is a well-known ferrimagnetic material with good durability at high temperatures and in erosive environments. Previous research has indicated that small Ti substitutions can enhance the coercivity at elevated temperatures. Our efforts aim at elucidating the underlying mechanism through measurements of electron energy loss magnetic chiral dichroism (EMCD), the electron analog to XMCD. We have deconvolved the Fe L-edges as obtained from classical EMCD measurements into different oxidation states of iron and estimated the influence of Ti substitution on the magnetic moments on each iron site. From this analysis, we identified that Ti2+ is substituted to the 4f2 site where Fe has an antiparallel magnetic moment in the Fe2+ octahedral oxidation state. However, EMCD signal of Fe2+ indicate parallel magnetic moment. EMCD measurements utilizing electron vortex beams (EVBs) in an aberration-corrected STEM hold the promise of achieving atomically resolved mappings of the magnetic moment. However, low signal-to-noise ratios (SNRs) currently impede atomic resolution in such measurements. Therefore, we have conducted EVB-EMCD measurements at the atomic scale using a direct detection camera. The impact on the method and achievable resolution will be discussed.

MA 46.49 Thu 15:00 Poster C

Size effect of the first-order magnetostructural transition in Ni-Mn-Sn — •Johannes Puy[1], David Koch[1], Enrico Bruder[1], Heiner Gutte[2], Volodymyr Baran[3], Konrad Opelt[1,4], Franziska Scheibel[1], and Oliver Gutfleisch[1] — [1]TU Darmstadt, Darmstadt, Germany — [2]TU Bergakademie Freiberg, Freiberg, Germany — [3]DESY P02.1, Hamburg, Germany — [4]Fraunhofer IWKS, Hanau, Germany

Ni-Mn-Sn Heusler alloys exhibit a first-order magnetostructural transition (FOMST) and a large magnetocaloric effect. The FOMST is driven by a nucleation and growth mechanism. A size dependence of the FOMST can be observed in powder. However, conventional milling induces defects despite annealing, so the defect and size dependencies are difficult to disentangle. In this study, spherical, gas-atomized, and homogenized Ni-Mn-Sn powders with different size fractions are used to investigate the size dependence of the FOMST. Magnetic, structural, and microstructural analyses show a decrease in transition width and an increase in thermal hysteresis with decreasing particle size. Temperature-dependent magnetometry on single particles shows a sharp, jump-like FOMST for particles below 50 μm, while a continuous FOMST is observed for particles above 50 μm. Temperature-dependent X-ray diffraction shows a complete FOMST for all size fractions. Electron backscatter diffraction shows an average grain size of 20 μm for all particles. Therefore, the size dependence of FOMST can be correlated with the single- and polycrystalline nature of the particles. We thank the CRC/TRR 270 "HoMMage" for funding.

MA 46.50 Thu 15:00 Poster C

Hybrid simulation tracing non-equlibrium spin-dynamics — •Lukas Jonda, Johan Briones, Sebastian T. Weber, Christopher Seibel, Sanjay Ashok, and Baerbel Rethfeld — Department of Physics and Research Center OPTIMAS, RPTU Kaiserslautern-Landau, Kaiserslautern

We simulate the interplay of several non-equilibrium phenomena aris-

ing in a magnetic film after femtosecond laser irradiation using a hybrid model. This approach consists of a combination of two methods: the μT model [1] and a kinetic Monte Carlo method [2]. The former treats the low-energetic electrons as ensembles, tracing spin-resolved temperatures and chemical potentials, as well as their gradients [3]. The latter traces the dynamics of individual high energetic non-equilibrium electrons, including spin-dependent scattering processes and a spin-flip probabilities. A model that can describe the transport of both the electronic ensemble and individual high-energy super-diffusive electrons is currently being developed. This allows the study of different types of non-equilibrium transport and their effects on magnetization dynamics.

References:
[1] B.Y. Mueller and B. Rethfeld, Phys. Rev. B, 90, 144420 (2014).
[2] J. Briones et al., J. Phys, 6, 035001 (2022).
[3] S. Ashok et al., App. Phys. Lett. 120, 142402 (2022).

MA 46.51 Thu 15:00 Poster C

Changes of the spin-spin and spin-lattice interaction induced by a ultrashort laser pulse — •Sergiy Mankovsky, Svitlana Polesya, and Hubert Ebert — Dept. Chemistry, LMU Munich, Butenandtstr. 11, D-81377 Munich, Germany

Ultrafast demagnetization implies complex dynamics concerning the electron, spin, and lattice degrees of freedom, coupled to each other and all being out-of-equilibrium after the laser pulse. The pure electron dynamics induced by a ultrashort laser pulse is well described within the time-dependent density functional theory (TD-DFT). However, spin and lattice excitations as well as interactions between all degrees of freedom are usually described making use of model Hamiltonians. The evolution of the spin system described using the Landau-Lifshitz-Gilbert equations is determined by the torque on the magnetic moments, stemming from different types of interactions entering the spin and spin-lattice Hamiltonian. The corresponding interaction parameters are determined by the electronic structure and can be calculated on a first-principles level. This implies that they should change together with the laser induced changes of the electronic structure. We will discuss the possible impact of such changes on the demagnetization dynamics, focusing on the isotropic exchange and different types of spin-lattice interactions. Their calculations have been performed employing TD-DFT potentials and occupation numbers generated by the Elk code [http://elk.sourceforge.net] for different time steps during the laser pulse and shortly after it. As is demonstrated for various systems, a strong modification of the parameters is found.

MA 46.52 Thu 15:00 Poster C

Static magnetic properties of ferromagnetic iron-nickel alloys in the Stoner model — •Sevim Kilic, Christopher Seibel, and Baerbel Rethfeld — Department of Physics and Research Center OPTIMAS, RPTU Kaiserslautern-Landau, Germany

In a previous work by Hofherr *et al.* [1], the direct, ultrafast and coherent spin transfer between subsystems of iron-nickel (NiFe) alloys through optical excitation (OISTR effect) was experimentally demonstrated. For this purpose, the spin-resolved density of states (DOS), which is essential for explaining the OISTR effect, was directly calculated using density functional theory (DFT). Now, we want to understand how well these spin-resolved DOS and their exchange splittings can be approximated with shifted paramagnetic density of states in the framework of the Stoner model.

Our research involves the investigation of paramagnetic density of states in NiFe alloys, which were determined by weighted averaging of pure iron and nickel DOS. The self-determined DOS were compared to DFT-calculated DOS of NiFe alloys from literature [2]. We then analyze the magnetization resulting from the application of the Stoner model to both model assumptions and compare it to the magnetization of Permalloy obtained from DFT calculations [3].

[1] M. Hofherr *et al.*, Sci. Adv. 6, 8717 (2020)
[2] http://compmat.org/electron-phonon-coupling/
[3] S. Sharma, MBI Berlin, private communication (2023)

MA 46.53 Thu 15:00 Poster C

Magnetization-dependent electronic structure and ultrafast electron dynamics in CrGeTe3 — •Túlio de Castro[1], Tommaso Pincelli[2], Lawson Lloyd[1], Maciej Dendzik[1], Shuo Dong[1], Samuel Beaulieu[1], Ralph Ernstorfer[2], and Laurenz Rettig[1] — [1]Fritz-Haber-Intitüt, Berlin — [2]Technische Universität, Berlin.

2D magnets present new possibilities to develop sizable and versatile nanodevices that work by manipulating the spin current, making it more efficient than charge-based devices. One of these promising 2D magnets is $CrGeTe_3$ (CGT) with a Curie temperature of $\approx$ 65K. Besides the magnetic order, the dimensionality allows us to study heterostructures with other 2D materials and make use of magnetic proximity effects. Here, we study bulk crystals of CGT using angle-resolved photoemission spectroscopy (ARPES) and femtosecond time-resolved ARPES (trARPES) to understand the magnetic-order induced changes to the electron distribution and the exchange splitting dynamics at different temperatures. By comparing data at the ASTRID synchrotron with data from our trARPES setup, we discuss the temperature-dependent band structure modifications and their ultrafast dynamics in bulk CGT. We further discuss the implication of our results for thin layers, monolayers, and heterostructures.

MA 46.54 Thu 15:00 Poster C

Magnetic order-dependent ultrafast magnetization dynamics in 4f-based intermetallics — •Abeer Arora[1], Yoav Will Windsor[5], Sang-Eun Lee[1], Daniela Zahn[1], Victoria Taylor[1], Hyein Jung[1], Túlio de Castro[1], Kristin Kliemt[2], Ch. Schüssler- Langeheine[3], Niko Pontius[3], Cornelius Krellner[2], Denis V. Vyalikh[4], and Laurenz Rettig[1] — [1]FHI der MPG, Berlin — [2]Phy. Inst., Goethe-Uni., Frankfurt am Main — [3]HZB für Materialien und Energie, Berlin — [4]DIPC, Basque, Spain — [5]IOAP, TU Berlin

The speed of magnetic devices is limited by the dissipation channels available for Angular Momentum Transfer (AMT). While demagnetization in ferromagnets (FMs) requires AMT to the lattice or spin transport, antiferromagnets (AFMs) offer potentially faster demagnetization through inter-sublattice AMT. Owing to the limited understanding of such channels, especially in 4f-based Lanthanides, we study the ultrafast magnetization dynamics in the $LnTm_2Si_2$ series of intermetallics (with Ln=Lanthanide, Tm=transition metal), with similar crystal structure and RKKY-mediated magnetic orders. We employ time-resolved resonant soft X-ray diffraction (trRXD) to study AFM compounds ($GdTm_2Si_2$, Tm=Co, Rh, Ir, $EuRh_2Si_2$), and trXMCD on Eu based FMs ($EuRu_2P_2$, $EuFe_2P_2$). The Gd series reveals a scaling of AMT rate with the 5d spin polarization of the conduction electrons, underscoring conduction electrons as an extra tuning parameter for Ln-based devices. Furthermore, a comparison of the AFM dynamics with Eu-FMs provides information about the AMT to the lattice.

MA 46.55 Thu 15:00 Poster C

Influence of transport mechanisms and film thickness on ultrafast magnetization dynamics and generation of spin-resolved charge currents — •Sanjay Ashok, Christopher Seibel, Sebastian T. Weber, and Baerbel Rethfeld — Department of Physics and Research Center OPTIMAS, RPTU Kaiserslautern-Landau

Generation of spin-resolved charge-currents and pure spin-currents in sub-picosecond timescales are pertinent to understand and employ ultrafast transport phenomena in spintronic device concepts. In this work we study the influence of transport mechanisms and film thickness on ultrafast magnetization dynamics using the thermodynamic μT model [1]. We also study the generation of spin-resolved charge currents as well as pure-spin currents in metallic ferromagnets.

We seperately simulate the influence of thermal-conductivity, electrical-conductivity, Seebeck effect and Peltier effect on ultrafast magnetization dynamics. We then study spin-resolved charge-currents and pure spin-currents at various depths of the material. We compare their relative magnitudes in Nickel films with various thicknesses.

Our simulations provide a framework to study the relative roles of various transport mechanisms in generation of ultrafast currents.

[1] Ashok et al. APL, 120 142402 (2022)

MA 46.56 Thu 15:00 Poster C

udkm1Dsim - A Python toolbox for simulating 1D ultrafast dynamics in condensed matter — •Daniel Schick — Max-Born-Institut für Nichtlineare Optik und Kurzzeitspektroskopie, Berlin, Germany

The udkm1Dsim toolbox is a collection of Python classes and routines to simulate the thermal, structural, and magnetic dynamics after laser excitation, as well as the corresponding light-scattering response in stratified (1D) samples, such as multilayers. The toolbox provides the capabilities to define arbitrary layered structures on the atomic level including a rich database of element-specific physical properties. The excitation of dynamics is represented by an N-temperature model

which is commonly applied in ultrafast physics. Structural dynamics due to thermal stresses are calculated by a linear-chain model of masses and springs. Magnetic dynamics can be calculated by a Landau-Lifschitz-Bloch or microscopic 3-temperature model. The resulting light-scattering response is computed by kinematical or dynamical X-ray theory which can also include polarization-dependent magnetic scattering. The udkm1Dsim toolbox is highly modular and allows for injecting user-defined inputs at any step within the simulation procedure.

MA 46.57 Thu 15:00 Poster C

The signature of 4f multiplet excitations to the M_5/M_4 branching ratio in Terbium and their influence on magnetization dynamics — •Beyza Salantur[1], Tim Amrhein[1], Niko Pontius[2], Christian Schuessler-Langeheine[2], Martin Weinelt[1], and Nele Thielemann-Kuehn[1] — [1]Freie Universität Berlin, Fachbereich Physik, Arnimallee 14, 14195 Berlin, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Albert-Einstein-Str. 15, 12489 Berlin, Germany

In $4f$-rare earth metals, magnetic order is established by intra- and interatomic exchange between $4f$ and $5d$ spins. We show that upon ultrafast optical excitation of the $5d$ electrons inelastic $5d$-$4f$ electron-electron scattering can alter the $4f$ orbital state and therewith the total angular momentum J [1]. This directly affects magneto crystalline anisotropy and has important implications for magnetization dynamics. Within a time-resolved X-ray absorption study at the FemtoSpeX slicing facility of BESSY II (HZB) we found transient changes of the M_5/M_4 branching ratio in Terbium, indicative of multiplet excitations changing J [2].

[1] N. Thielemann-Kühn et al., *Optical control of 4f orbital state in rare-earth metals.* https://doi.org/10.48550/arXiv.2106.09999 (Science Advances, in revision)

[2] B. T. Thole and G. van der Laan., *Branching ratio in x-ray absorption spectroscopy.* Phys. Rev. B, 38:3158-3171, Aug 1988.

MA 46.58 Thu 15:00 Poster C

Differentiating mechanisms that drive ultrafast magnetization precession — •Fried-Conrad Weber[1], Jasmin Jarecki[2], Max Mattern[1], Alexander von Reppert[1], and Matias Bargheer[1,3] — [1]Institute of Physics and Astronomy, University of Potsdam — [2]Max-Born-Institute, Berlin — [3]Helmholtz-Zentrum, Berlin

We study the influence of strain and heat on the ultrafast magnetization precession in Cobalt and Nickel. To achieve this, we combine trMOKE measurement of various samples under different initial conditions, with numerical simulations. We model the ultrafast dynamics of heat and strain in laser-excited thin films and the magnetization precession that is triggered by the concomitant time-dependent effective fields. In this way, we aim at understanding and controlling the complex interplay of heat, strain and magnetization dynamics.

MA 46.59 Thu 15:00 Poster C

Theoretical study of optical excitation effects in RuO_2 — •Luca Haag[1], Marius Weber[1], Kai Leckron[1], Stephan Wust[1], Benjamin Stadtmüller[1], Libor Šmejkal[2], Jairo Sinova[2], and Hans Christian Schneider[1] — [1]Department of Physics and Research Center OPTIMAS, University of Kaiserslautern-Landau, 67633 Kaiserslautern, Germany — [2]Institut für Physik, Johannes Gutenberg University Mainz, 55099 Mainz, Germany

We study theoretically the optical response of the d-wave altermagnet RuO2. As an altermagnetic material RuO2 shows a momentum-dependent spin polarization in reciprocal space without net magnetization [1,2]. We investigate in particular how the underlying symmetries affect its optical characteristics. We employ a hybrid approach that combines Density Functional Theory (DFT) and optical transition probabilities in a Fermi's Golden Rule approach [3] to simulate the excitation with momentum, spin and band resolution.

[1] L. Šmejkal et al., Phys. Rev. X 12, 040501 (2022)
[2] L. Šmejkal et al., Phys. Rev. X 12, 011028 (2022)
[3] S. Essert and H. C. Schneider, Phys. Rev. B. 84, 224405 (2011)

MA 46.60 Thu 15:00 Poster C

Studying all-optical magnetization switching of GdFe by double-pulse laser excitation — Rahil Hosseinifar[1], Ivar Kumberg[1], Felix Steinbach[2], •Sangeeta Thakur[1], Sebastien E. Hadjadj[1], Jendrik Gördes[1], Mario Fix[3], Josè Miguel Lendìnez[4], Chowdhury Awsaf[1], Manfred Albrecht[3], Florian Kronast[5], Unai Atxitia[4], Clemens von Korff Schmising[2], and Wolfgang Kuch[1] — [1]Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — [2]Max Born Institute for Nonlinear Optics and Short Pulse Spectroscopy, Max-Born Straße 2A, 12489 Berlin, Germany — [3]Institut für Physik, Universität Augsburg, Universitätsstraße 1, 86159 Augsburg, Germany — [4]Instituto de Ciencia de Materiales de Madrid, CSIC, Cantoblanco, 28049 Madrid, Spain — [5]Helmholtz-Zentrum Berlin, Albert-Einstein-Straße 15, 12489 Berlin, Germany

We performed double-pulse experiments on a $Gd_{26}Fe_{74}$ ferrimagnetic alloy with a magnetic compensation temperature of about 120 K by x-ray magnetic circular dichroism photoelectron emission and optical Kerr microscopy. We demonstrate the effects of different ratios of fluence between two single laser pulses of 800 nm wavelength and a duration of 120 and 250 fs, at 70 K and at room temperature. We identified a time delay between 3 and 20 ps at which all-optical switching is suppressed. Atomistic spin dynamics (ASD) simulations have been carried out to describe the non-equilibrium dynamics following the excitation. They successfully describe the behaviour of the switching as a function of laser fluences and time delay between the two pulses.

MA 46.61 Thu 15:00 Poster C

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

Controlling the magnetic state of 2D materials is a key enabler for spintronics. Especially in the novel class of non-van der Waals 2D compounds – materials derived from non-layered bulk counterparts – promising (surface) magnetic properties were outlined in recent years [1,2]. Utilising data-mining and autonomous density functional theory calculations, we demonstrate the modification of magnetic properties of these materials by hydrogen passivation [3]. The magnetic configurations are tuned to states with flipped and enhanced moments, which we rationalize by analysing Bader charges. For 2D $CdTiO_3$ – a diamagnetic compound in the pristine case – we observe an onset of ferromagnetism upon hydrogenation. Further investigation of the magnetization density in both pristine and passivated systems provides a detailed analysis of modified local spin symmetries and the emergence of ferromagnetism. Our results suggest that selective surface passivation is a powerful tool for tailoring magnetic properties of nanomaterials, such as non-vdW 2D compounds.

[1] R. Friedrich *et al.*, Nano Lett. **22**, 989 (2022).
[2] T. Barnowsky *et al.*, Adv. Electron. Mater. **9**, 2201112 (2023).
[3] T. Barnowsky *et al.*, submitted, arXiv:2310.07329 (2023).

MA 46.62 Thu 15:00 Poster C

Interfacial Engineering of ultrafast dynamics in 2d ferromagnets — •Nele Stetzuhn[1,2], Clemens von Korff Schmising[2], Nikola Nedeljkovic[1], Stefan Eisebitt[2], and Kirill I. Bolotin[1] — [1]Freie Universität Berlin, Arnimallee 14, 14195 Berlin — [2]Max-Born-Insitut, Max-Born-Straße 2A, 12489 Berlin

The clean and atomically sharp interfaces of 2d materials offer a convenient way to manipulate their properties by introducing, e.g., screening, external fields or doping. In this work, we investigate whether it is possible to influence de- and remagnetization dynamics in the 2d ferromagnet Fe3GeTe2 by varying its substrate between hBN and graphene, as well as suspending it over a cavity. Differences in recovery times of up to a factor 10 have been estimated from simulations between a supported and a suspended device. We test this theoretical prediction using time- and spatially resolved Kerr microscopy.

MA 46.63 Thu 15:00 Poster C

Classification of complex 2D magnetic ground states using unsupervised Contrastive Learning — Jannis Neuhaus-Steinmetz[1], •Tim Matthies[1], Elena Y. Vedmedenko[1], Thore Posske[2], and Roland Wiesendanger[1] — [1]Department of Physics, University of Hamburg, Hamburg, Germany — [2]I. Institute for Theoretical Physics, University of Hamburg, Hamburg, Germany

Phase diagrams capture the essential features of a system in many areas of physics. Distinguishing one phase from another is often done by hand-crafted selection rules and an automated approach could accel-

erate this process. Here, we use a machine learning technique called contrastive learning to classify 18,000 magnetic ground state configurations into 12 distinct clusters. This is done by using a hybrid approach of increasing the number of clusters given by the model to 40 and then merging these clusters into the 12 phases by hand. The ground states of two-dimensional magnetic atomic lattices on metallic substrates are generated by fitting a tight-binding model to a classical Heisenberg model and subsequent classical Monte Carlo calculations. The symmetries of the system are utilized as transformations to cluster identical phases together. Furthermore, we investigate the representation space created by the model as a quick overview for understanding large amounts of physical data. The approach contributes to a better understanding of the connection between magnetism and topological electronic matter. Our results are generalizable to other systems in condensed matter physics and beyond.

MA 46.64 Thu 15:00 Poster C

Implementation of spin-torque exchange-correlation functionals in VASP for noncollinear magnetism — •Fabien Tran, Marie-Therese Huebsch, and Martijn Marsman — VASP Software GmbH, Vienna, Austria

The implementation in VASP of an exchange-correlation functional for noncollinear magnetism is reported. It is the functional developed by Tancogne-Dejean, Rubio and Ullrich [Phys. Rev. B **107**, 165111 (2023)], based on the idea of Pittalis, Vignale and Eich [Phys. Rev. B **96**, 035141 (2017)]. The functional is of the meta-GGA type since it depends on the kinetic-energy density and Laplacian of the density. However, it also depends on the paramagnetic current density and, furthermore, on the full 2×2 spin density matrix, therefore leading to a non-zero exchange-correlation spin torque. The results of calculations on noncollinear systems (e.g. bulk Mn_3Sn and the Cr_3 molecule) are reported and compared to results obtained with standard functionals, e.g. PBE and SCAN.

MA 46.65 Thu 15:00 Poster C

Ferromagnetic resonance simulations of arranged magnetic nanoparticles — •Felix Schug[1,2], Nils Neugebauer[2,3], Michael Czerner[1,2], and Christian Heiliger[1,2] — [1]Institute for Theoretical Physics, Justus Liebig University Giessen, Heinrich-Buff-Ring 16, 35392 Giessen, Germany — [2]Center for Materials Research (LaMa), Justus Liebig University Giessen, Heinrich-Buff-Ring 16, 35392 Giessen, Germany — [3]Institute of Experimental Physics I, Justus Liebig University Giessen, Heinrich-Buff-Ring 16, 35392 Giessen, Germany

Magnetic nanoparticles (MNPs) are utilized in a variety of electronic applications due to their unique magnetic characteristics. *Mesocrystals*, composed of arranged MNPs, offer additional degrees of freedom to manipulate these magnetic characteristics. Understanding the magnetic properties of mesocrystals is crucial for optimizing their use in applications. In this study, we used the publically available micromagnetic simulation tool OOMMF, to investigate mesocrystals composed of magnetite MNPs. We arranged the mesocrystals on a periodic grid with varying inter-mesocrystal distances by employing two-dimensional periodic boundary conditions. Our simulations of ferromagnetic resonance (FMR) spectra revealed various resonance frequencies. A spatially resolved analysis was conducted to investigate the origins of these frequencies within the mesocrystal.

MA 46.66 Thu 15:00 Poster C

An Ab Initio Study of Monolayer Mn2Mg2X5 (X = S, Se), a Novel Family of 2D Half-Metallic Ferromagnets — •Soheil Ershadrad and Biplab Sanyal — Uppsala Univeristy, Uppsala, Sweden

Based on first principle calculations, we propose a family of stable 2D ferromagnets, Mn2Mg2X5 (X = S, Se), with a half-metallic electronic structure. They possess a high Curie temperature, and strong magnetocrystalline anisotropy. An indirect exchange interaction, mediated by chalcogen atoms, dominates in these crystals. Their half-metallicity and high-temperature magnetism render them suitable candidates for spintronic applications.

MA 46.67 Thu 15:00 Poster C

Hopf index calculation in micromagnetic finite-element simulations — •Louis Gallard[1], Karin Everschor-Sitte[2], and Riccardo Hertel[1] — [1]Université de Strasbourg and CNRS, IPCMS, 67000 Strasbourg, France — [2]Faculty of Physics and CENIDE, University of Duisburg-Essen, 47057 Duisburg, Germany

Magnetic Hopfions are complex topological textures that can be regarded as three-dimensional (3D) counterparts of skyrmions. They have recently attracted considerable interest due to their intriguing structure and possible use in spintronic devices. Unlike skyrmions, which are usually easy to spot in magnetic configurations, Hopfions are difficult to identify because of their complex knotted 3D vector field distribution. The difficulty arises even in micromagnetic simulations, where detailed information about the magnetic structure is readily available. The Hopf index, a topological invariant, provides a measure of Hopfions that allows for their quantitative detection. However, in the general case of 3D samples of finite size, calculating the Hopf index usually involves a two-fold volume integral, whose $\mathcal{O}(N^2)$ scaling makes its evaluation impracticable in large-scale computations. Here, we present an alternative approach which involves solving a partial differential equation by using a hybrid finite-element / boundary-element method. We retain a scaling of nearly $\mathcal{O}(N)$, which is suitable for high-performance computing. The method is fast enough to be used during dynamic micromagnetic simulations to monitor the Hopf index's evolution in time. We demonstrate the application of the method to a Hopfion structure in a cylinder and a torus geometry.

MA 46.68 Thu 15:00 Poster C

The effectiveness of spin injection from bulk Nickel into phosphorene — •Puja Kumari and Soumya Jyoti Ray — Indian Institute of Technology Patna, Bihar, India, 801106

The moderate electronic band gap and larger carrier mobility of 2D phosphorene, make it a promising candidate for future nanoelectronics. With the addition of magnetism to black phosphorene, its applications will be greatly expanded, as well as creating the possibility to design new spintronic devices. Here employing first-principles calculations, we investigate the efficiency of spin transmission from a ferromagnetic electrode (Ni) into phosphorene (P/Ni(111)). Additionally, enhance the spin injection efficiency (SIE) by replacing a single phosphorene layer with bi- and tri-layers of phosphorene. Twist engineering allows us to moderate the SIE up to 60%. To begin with, we systematically studied the structural, electronic, and magnetic properties of the P/Ni(111) junction including bi- and tri-layers of phosphorene. The mono-, bi-, and tri- layers of phosphorene on the Ni surface exhibit metallic properties upon establishing ohmic contact, demonstrating a proximity effect. After that, we have done a detailed analysis of the transport property of spin carriers with negative differential resistance. The findings of our study provide new insights into the design of phosphorene-specific spin devices.

MA 46.69 Thu 15:00 Poster C

Ab-initio spin dynamics in non-collinear magnets — •David Eilmsteiner[1,2], Pawel Buczek[2], and Arthur Ernst[1] — [1]Johannes Kepler University, Linz, Austria — [2]HAW Hamburg, Hamburg, Germany

The investigation of magnetization dynamics is a highly active field of research on both the experimental and the theoretical side. Our group focuses on the determination of magnetic properties by means of the Korringa-Kohn-Rostoker Green's functions approach to density functional theory. This method not only allows for the self-consistent determination of ground state properties of ordered and disordered materials, it can also conveniently be extended to the description of magnetization dynamics in the linear response regime, which allows for the investigation of various magnetic excitations, such as Stoner excitations or magnons on an equal footing.

On my poster, I will focus on our current effort to extend our method to non-collinear magnetic systems. Investigating the dynamics of non-collinear magnets, stabilized either by geometric frustration or relativistic effects, is of great interest as, in that case, the magnetization dynamics are no longer decoupled from charge density oscillations. Furthermore, the spin-flip excitations are not decoupled from the longitudinal magnetization dynamics. These effects open additional decay channels for spin dynamics, which are absent in the collinear case.

MA 46.70 Thu 15:00 Poster C

An iterative approach for the coupling of surface acoustic waves to micromagnetics — •Michael Karl Steinbauer[1], Peter Flauger[1], Bernhard Emhofer[1], Matthias Küss[2], Stephan Maximilian Glamsch[2], Matthias Volz[3], Hubert Krenner[3], Manfred Albrecht[2], and Claas Abert[1] — [1]University of Vienna — [2]University of Augsburg — [3]University of Münster

In recent years, the coupling of magnetic and phononic systems has emerged as a rapidly developing field of study. As these interactions

usually happen with a resonance frequency in the GHz regime, it has a variety of possible industrial applications [1].

In many experimental publications, a macro-spin model has been used to simulate the influence of surface acoustic waves (SAWs) onto the magnetic system. [2]. However, this approach is not capable of accurately predicting the magnetization dynamics in systems with spatially varying magnetization patterns such as magnetic domains.

In this work, we present a micromagnetic model, which is able to simulate these interactions using an extension of the magnum.np python library [3]. Additionally, we introduce an iterative algorithm to predict the decay of the SAW amplitude as it travels along a magnetic structure.

[1] P. Delsing et al., J. Phys. D: Appl. Phys. 52, 353001 (2019).
[2] M. Küß et al., Phys. Rev. Appl. 15, 034046 (2021).
[3] F. Bruckner et al., Sci. Rep. 13, 12054 (2023).

MA 46.71 Thu 15:00 Poster C

Origin of Magnetism in monolayer VI3 — •Anita Francis and Swapan Pati — JNCASR, Bengaluru, India

We have studied the magnetic properties of monolayer VI3 from first principles. Using the generalised Heisenberg model we have calculated the isotropic and anisotropic exchange parameters for the system, which we then have used in a Monte Carlo simulation to predict the ordering temperature in the system. We observe that the system orders ferromagnetically at a temperature around 50K.

MA 46.72 Thu 15:00 Poster C

Antiferromagnetically coupled half-shell magnetite nanoparticles with tuneable magnetic remanence — •Patrick Steinkraus[1], Inci Nur-Sahin[1], Veronica Salguerino[2], Ecem Tiryak[2], Marina Spasova[1], and Michael Farle[1] — [1]Faculty of Physics and Center of Nanointegration (CENIDE), University of Duisburg-Essen, Duisburg, 47057 Germany — [2]Departamento de Física Aplicada and CINBIO, Universidade de Vigo, 36310 Vigo, Spain

Magnetite nano-hybrids were chemically synthesized in the form of two magnetite half-shells with a length of 460 nm and width of 90 nm covered with a 30 nm thick silicon dioxide layer. Structure, chemical composition, and morphology were characterized using Transmission Electron Microscopy, Energy Dispersive X-Ray Spectroscopy and Electron Energy Loss Spectroscopy. The magnetic hysteresis of individual particles was simulated using data from our structural and morphological analysis. In the absence of magnetic field, the composite particle acts like an antiferromagnet. However, when exposed to an external magnetic field of B = 75mT, the magnetizations of the two half-shells align ferromagnetically. Below B = -34mT, the magnetizations revert to their antiparallel alignment. The 30 nm thick silica shell suppresses the dipole-dipole interaction between particles preventing their agglomeration. These properties may make these nanoparticles perfect candidates for magneto-mechanical and hyperthermia therapies. Funding by the European Union's Horizon 2020, project No 857502 (MaNaCa) is gratefully acknowledged.

MA 46.73 Thu 15:00 Poster C

Quantum Tunneling of Magnetization in Tilted Toroidal Systems — •Jonas Waltenberg and Jürgen Schnack — Bielefeld University

Molecular magnets with a toroidal arrangement of the easy anisotropy axes are often viewed as promising candidates for magnetic storage and quantum computing [1,2]. For this a high stability against perturbations like external magnetic fields is needed. As a measure of this stability the tunneling matrix elements for spin systems of different sizes with easy anisotropy axes tilted from the collinear arrangement to the toroidal arrangement are calculated. It is discussed which systems are stable against this quantum tunneling of magnetization.

[1] D. Pister, K. Irländer, D. Westerbeck, J. Schnack, Toroidal magnetic molecules stripped to their basics, Phys. Rev. Research 4 (2022) 033221

[2] K. Irländer, J. Schnack, Studies of decoherence in strongly anisotropic spin triangles with toroidal or general non-collinear easy axes, Phys. Rev. Research 5 (2023) 013192

MA 46.74 Thu 15:00 Poster C

A study of magnetic properties of face-sharing 3d manganese trimers — •Anzar Ali[1,2], Sungkyun Choi[1], and Masahiko Isobe[2] — [1]Sungkyunkwan University, Suwon 16419, Republic of Korea — [2]Max Planck Institute for Solid State Research, Stuttgart Germany 70569

The emergence of a potentially conflicting molecular orbital state in correlated electron systems has recently garnered substantial attention in condensed matter physics, presenting a promising arena for uncovering novel electronic phases. Although this state has predominantly been explored in 4d and 5d transition metal oxides due to their extended orbital nature, our investigation focuses on 3d transition metal-based compounds featuring a face-sharing trimer. This study unveils systematic findings and a comprehensive understanding of two new 3d hexagonal perovskites, Ba4TaMn3O12 and Ba4NbMn3O12, wherein a face-sharing Mn trimer along the c-axis interacts within the hexagonal lattice. Surprisingly, effective magnetic moments suggest an S=2 trimer, while magnetic entropies propose a localized S=3/2 trimer. This apparent contrast finds resolution in a partial molecular orbital state, combining antiferromagnetically localized moments (S=3/2) and a delocalized one-electron (S=1/2) state within the trimer.

Ab-initio calculations reveal itinerant electron sharing and AF ordering in a Mn trimer, resulting in a unique coexistence of localized and delocalized electron states in a 3d material. To eliminate powder limitations, we stress the importance of growing single crystals using floating zone techniques to address disorder and impurity phases.

MA 46.75 Thu 15:00 Poster C

Probing spin-orbit coupling at hybrid single-molecule magnet/metal interfaces — •David Anthofer[1], Ashish Moharana[1], Dominik Laible[2], Fabian Kammerbauer[1], Eva Rentschler[2], and Angela Wittmann[1] — [1]Institut für Physik, Johannes-Gutenberg Universität Mainz, 55128 Mainz, Deutschland — [2]Department Chemie, Johannes-Gutenberg Universität Mainz, 55128 Mainz, Deutschland

Single-molecule magnets have recently gained significant interest for their ability to retain magnetic information at the molecular level, surpassing the superparamagnetic limit of conventional magnetic storage technologies and offering potential applications in ultra-compact and high-density data storage devices. A crucial challenge hindering their application in technology is the integration with thin-film devices. To master this challenge, we explore the spin-orbit coupling in hybrid single-molecule magnet/non-magnetic metal thin film heterostructures to understand the impact of hybridization. For this, we inject a pure spin current at ferromagnetic resonance into the hybrid interface, allowing us to measure the spin-to-charge conversion efficiency. In this work, we utilize single-molecule magnets based on the metallacrown system, chosen for their unique combination of reliability and versatility. Quantifying the adsorption for molecular systems with different constitutions and planarity allows us to conclude the impact of molecular structure on the effective spin-orbit coupling and magnetic coupling at the hybrid interface, paving the path toward novel spintronic devices.

MA 46.76 Thu 15:00 Poster C

Computational Study of the Magnetic Properties of Simple Molecules Containing Boron-Boron Bonds — •Ljubica Dimova and Irina Petreska — Ss. Cyril and Methodius University in Skopje, Faculty of Natural Sciences and Mathematics, Institute of Physics, Skopje, Macedonia

Our results from the computational studies of the spin properties of some selected paramagnetic molecular species will be presented. Experimentally, the properties of the paramagnetic molecules are investigated by the electron paramagnetic resonance (EPR) spectroscopy, which is usually complemented by the density functional theory (DFT). DFT plays a significant role in prediction of the molecular magnetic properties, as well as in the rationalization of the experimentally observed EPR spectra. We start our DFT study with the diboron molecule, as a simple example, found in a triplet ground state, due to the two unpaired electrons. Further, we extend our analysis to more complex compounds, containing boron-boron bonds, aiming at investigation of the effects of the surrounding. In particular, we evaluate the **g**-tensor values, including the relativistic mass correction, diamagnetic correction, orbital Zeeman and spin-orbit coupling contributions. For this purpose, we employ the GIAO (Gauge-Independent Atomic Orbital) method to fully optimised structures at various levels of theory. The obtained results are analysed in detail and compared with the existing experimental data.

MA 46.77 Thu 15:00 Poster C

Laser-induced generation of magnetic fields on an ultrafast timescale — •Hannah Bendin, Benjamin Schwager, and Jamal Berakdar — Martin-Luther-Universität Halle-Wittenberg

Enabling ultrafast switching of magnetic moments on a nanoscopic scale is an important step on the path to minimization of electronic devices. Therefore, finding new ways of generating the respective magnetic fields is essential. In this project, the possibility of utilizing endohedral fullerenes for those purposes is investigated. Fullerenes possess superatom molecular orbitals (SAMOs). For the buckminsterfullerene, those diffuse excited states are similar in structure to hydrogen orbitals while being on a nanometer scale. Using an optical vortex beam to excite electrons and transfer spin as well as orbital angular momentum, charge currents can be generated in the SAMOs. The induced magnetic field inside the cage of the fullerene and the spin manipulation of enclosed atoms are investigated.

MA 46.78 Thu 15:00 Poster C

Magnetocalorics for spin systems with dipolar interaction — •Dennis Westerbeck and Jürgen Schnack — Bielefeld University

For the development of new coolants for the low temperature cooling, it is necessary to take a look at the influence of the inevitable dipolar interaction on the cooling efficiency. We investigated small spin systems with common shapes like rings, tetrahedrons and butterflys, to search for areas, where the dipolar interaction has the most favourable effect on important thermodynamic variables

MA 46.79 Thu 15:00 Poster C

Probing the magnetic behavior of the metastable high-spin state achieved by light-induced excited spin-state trapping in Fe (II) complexes — •Marcel Walter[1], Tarek Al Said[2], Clara W.A. Trommer[3], Torben Adam[3], Felix Tuczek[3], Karsten Holldack[2], Wolfgang Kuch[1], and Sangeeta Thakur[1] — [1]Freie Universität Berlin, Institut für Experimentalphysik, 14195 Berlin, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie, 12489 Berlin, Germany — [3]Institut für Anorganische Chemie, Christian-Albrechts Universität zu Kiel, 24098 Kiel, Germany

The magnetic behavior of the metastable high-spin (HS) state of the binuclear iron complex $[(Fe(H_2B(pz)_2)_2)_2$ (μ-bipy-ac-bipy)] and the mononuclear complex $[Fe(H_2B(pz)_2)_2$(bipy)] was investigated at 5 K by electron paramagnetic resonance (EPR) spectroscopy in a magnetic field of 1-10 T. The relaxation time of the spins from the low-spin state to reach the metastable HS state after light-induced excited spin state trapping is faster for the binuclear complex (11 min) as compared to the mononuclear complex (16 min). The spin Hamiltonian parameters obtained from a simulation of the magnetic field map of the EPR measurements indicate a large value of zero-field splitting (ZFS) for both complexes, which can be explained by the contribution of spin-orbit coupling to the ZFS during the decay of the excited singlet states $^1T_{1g}$ to the excited $^5T_{2g}$ metastable HS state.

MA 46.80 Thu 15:00 Poster C

Submonolayer films of tridentate spin-crossover molecules with high transition temperatures deposited on graphite — •Jorge Torres[1], Sangeeta Thakur[1], Sascha Ossinger[2], Jan Grunwald[2], Ivar Kumberg[1], Evangelos Golias[3], Clara W.A. Trommer[2], Sebastien Hadjadj[1], Marcel Walter[1], Jendrik Gördes[1], Rahil Hosseinifar[1], Pin-Chi Liu[1], Tauqir Shinwari[1], Chen Luo[4], Lalminthang Kipgen[1], Florin Radu[4], Felix Tuczek[2], and Wolfgang Kuch[1] — [1]Freie Universität Berlin, Berlin, Germany — [2]Christian-Albrechts Universität zu Kiel, Kiel, Germany — [3]MAX IV Laboratory, Lund, Sweden — [4]Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany

Spin-crossover molecules (SCM) are organic metal complexes the spin states of which can be changed from low-spin (LS) to high-spin (HS) by stimulation with light, temperature or pressure. Here, we use x-ray absorption (XAS) and differential reflectance (DRS) spectroscopies to study bulk and submonolayer coverages of sublimable tridentate SCM's on graphite. Submonolayer films of $[Fe\{H_2B(pz)(pypz)\}_2]$, which can exist in two different polymorphic structural phases, exhibit a transition temperature ($T_{1/2}$) around 300 K. For the nominal LS complex $[Fe\{pypypyr\}_2]$ ($T_{1/2}$ above 510 K), XAS bulk measurements show a long-lived low-temperature HS state. Finally, $[Co\{H_2B(pz)(pypz)\}_2]$ and $[Co\{dpzca\}_2]$ show a reduced light-induced excited spin-state trapping (LIESST) efficiency compared to the thermally driven spin transition. From these results, a link between polymorphic phases and LIESST temperatures as a function of film thickness might exist.

MA 46.81 Thu 15:00 Poster C

Chiral Induced Spin Selectivity Effect at Helical Molecule-metal Interfaces — •Ashish Moharana[1], Hao Wu[2], Shuanglong Wang[2], Fabian Kammerbauer[1], Maria-Andromachi Syskaki[1], Zijie Qiu[2,3], Tomasz Marszalek[2], and Angela Wittmann[1] — [1]Institut für Physik, Johannes-Gutenberg-Universität Mainz, 55099 Mainz, Germany — [2]Max Planck Institute for Polymer Research, Ackermannweg 10, 55128, Mainz, Germany — [3]School of Science and Engineering, Shenzhen Institute of Aggregate Science and Technology, The Chinese University of Hong Kong, Shenzhen, 518172, P.R. China

The observation of spin-dependent transmission of electrons through chiral molecules has led to the discovery of chiral-induced spin selectivity (CISS). The high efficiency of the spin filtering effect in chiral molecules has recently gained significant interest due to the high potential for novel hybrid molecule magnetic spintronics applications. However, the fundamental mechanisms underlying the CISS effect at the molecule-metal interface remain not entirely understood. In our work, we explore spintronic phenomena at hybrid chiral molecule magnetic interfaces to elucidate the underlying mechanisms of the chiral-induced spin selectivity effect. For this, we investigate the spin-to-charge conversion efficiency in chiral molecule/ metallic thin film heterostructures. This study focuses on the impact of the adsorption of chiral molecules on the spin-to-charge conversion at the molecule-metal hybrid interface. Quantifying the impact as a function of the molecular structure of the chiral molecules will reveal the role of the structural design in the spin-filtering effect.

MA 46.82 Thu 15:00 Poster C

Density-functional studies of $CuCu_4$ metallacrowns deposited on gold surfaces — •Ariyan Tavakoli, Benedikt Baumann, Stefan Lach, Benjamin Stadtmüller, Christiane Ziegler, and Hans Christian Schneider — Physics Department, RPTU Kaiserslautern-Landau, KaiserslauternGermany

We present ab-initio calculations for the electronic and magnetic properties of CuCu4 metallacrowns [1] adsorbed on an Au (111) surface for different deposition methods. In the framework of the VASP code, we compare gas-phase results obtained using DFT and DFT+U calculations, and investigate the DOS and ligand structure of the different hybridized systems.

[1] P. Happ et al., Phys. Rev. B 93, 174404 (2016).

MA 46.83 Thu 15:00 Poster C

Magnetic structure of $Cu(tn)Cl_2$ molecular magnet — •Jakub Šebesta[1], Dominik Legut[1], Robert Tarasenko[2], Olha Vinnik[2], Erik Čižmár[2], Jozef Strečka[2], Martin Orendáč[2], and Alžbeta Orendáčová[2] — [1]IT4Innovations, VŠB-TU Ostrava, 17.listopadu 2172/15, 708 00 Ostrava, Czech Republic — [2]Institute of Physics, P. J. Šafárik University, Park Angelinum 9, 04001 Košice, Slovakia

Magnetic materials have long been the subject of scientific inquiry. Nevertheless, the research started to expand its focus beyond aiming at low-dimensional systems. Exploring beyond the traditional bulk magnets could bring innovations thanks to different confinement resulting in unique physical properties. Apart from layer materials, molecular magnets are significant representatives. In this work, we are discussing an organo-metallic $Cu(tn)Cl_2$ quantum magnet bearing a 2D layered magnetic structure. Combining DFT calculations with an evaluation of magnetic exchange interactions, we discuss the magnetic complex structure and show the strong dependence of the magnetic properties on molecular conformation. It includes not only the variation of the magnetic exchange but also the modification of the magnetic state itself.

MA 46.84 Thu 15:00 Poster C

On the magnetocaloric effect of terbium in high fields — •Tino Gottschall[1], Michael Kuz'min[2], Eduard Bykov[1], Deborah Schlagel[3], Yaroslav Mudryk[3], and J. Wosnitza[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf — [2]Aix-Marseille Université, France — [3]Ames Laboratory, U.S. Department of Energy, USA

Magnetic cooling is a refrigeration technique that is based on the so-called magnetocaloric effect, the change of temperature caused by a magnetic field. It can be utilized to construct environmentally friendly cooling devices, air conditioners, and heat pumps. The element gadolinium plays a special role in this context, as it has an extraordinary large magnetocaloric effect at room temperature. In this presentation, however, we would like to focus on another rare-earth element, namely terbium. We show on a single crystal that it even outperforms gadolinium in terms of the adiabatic temperature change in high pulsed magnetic fields. Due to the extremely strong magnetic anisotropy, we have also observed an enormous rotational

magnetocaloric effect, which could be interesting for the development of future magnetic-cooling devices.

MA 46.85 Thu 15:00 Poster C

Estimation of the conventional giant barocaloric effect in $Ni_{50}Mn_{34.8}In_{14.2}B$ — •Sven Wiesekopsieker[1,2], Tapas Samanta[1], Chris Taake[1], Laila Bondzio[1], Andreas Hütten[1], and Luana Caron[1,2] — [1]Faculty of Physics, Bielefeld University, Bielefeld 33501, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin 12489, Germany

Heusler alloys such as NiMn(In, Ga, Sn)-based systems are of special interest because they display a magnetostructural transition of first-order, necessary for a large barocaloric effect (BCE)[1]. The off-stoichiometric Heusler alloy $Ni_{50}Mn_{34.8}In_{14.2}B$ shows a martensitic phase transition from a low T, low moment martensitic phase with monoclinic structure to a high T, ferromagnetic austenite phase with cubic L21 structure. We have studied the BCE in this compound using a combination of magnetic measurements under hydrostatic pressure and differential scanning calorimetry at 1 atm. Application of a pressure up to 8.2 kbar shifts the transition from 305 K up to 327 K and decreases thermal hysteresis from ca. 6.5 to 4.5 K at $\mu_0 H = 7$ T. This, combined with a large transition entropy change of $|\Delta S_{tr}| = 35$ J/(kg K), results in a decent refrigeration capacity which, compared to similar systems such as $Ni_{58.3}Mn_{17.1}Ga_{24.6}$ with $\Delta T_{hyst} = 11$ K and $|\Delta S_{tr}| = 16$ J/(kg K) [2], or $Ni_{44.6}Co_{5.5}Mn_{35.5}In_{14.4}$ with $\Delta T_{hyst} = 19$ K and $|\Delta S_{tr}| = 16$ J/(kg K) [1], represents a large improvement.

[1] X. J. He et al., J. Scri. Mater. 145, 58 (2018)
[2] X. J. He et al., J. Mater. Sci. 52, 2915 (2017)

MA 46.86 Thu 15:00 Poster C

Anomalous Nernst effect in Ge-substituted iron nitride thin films — •Jakub Vit[1], Petr Levinsky[1], Kyo-Hoon Ahn[1], Marketa Jarosova[1], Imants Dirba[2], and Karel Knizek[1] — [1]Institute of Physics, Czech Academy of Sciences, Prague, Czechia — [2]TU Darmstadt, Germany

Iron nitrides – composed of abundant elements – have Curie temperatures (T_C) well above the room temperature, below which they exhibit the anomalous Nernst effect (ANE) larger than pure iron. [1] Our recent DFT calculations suggested that the ANE may be further increased by substitution of other elements for iron. [2] Nevertheless, synthesis of such theoretically predicted compounds may be complicated. One of few successful syntheses of substituted iron nitrides is the case of $Fe_{4-x}Ge_xN$ (x=0 – 1) antiperovskites, which were characterized in a form of powder. [3] We investigated the same compounds grown as epitaxial thin films, which provides convenient geometry for thermoelectric applications. Upon Ge-doping, T_C expectedly decreases and the cubic structure becomes tetragonal. We measured magnetic properties, resistivity and the Nernst effect, the latter changing sign upon varying Ge content with comparable magnitude to Fe_4N. This was reproduced in our DFT calculations when selecting the on-site Coulomb repulsion parameter U=1 eV, showing that finite U is necessary to use despite broad bands, typical for nitrides.

[1] S. Isogami et al., *Appl. Phys. Express*, **10**, 073005 (2017)
[2] K.-H. Ahn et al., *Phys. Rev. B*, **108**, 075123 (2023)
[3] T. Scholz and R. Dronskowski, *J. Mater. Chem. C*, **5**, 166 (2017)