MA 45: Computational Magnetism

Time: Friday 9:30–12:30 Location: H18

MA 45.1 Fri 9:30 H18

Magnetic Interactions and Spin Coupling in Endohedral Fullerene Nanostructures — •Arkamita Bandyopadhyay and Jamal Berakdar — Martin-Luther-Universität Halle-Wittenberg, Karl-Freiherr-von-Fritsch-Str. 3 06120 Halle/Saale

Our work investigates the spin-spin interactions in endohedral fullerene clusters, with a particular focus on the effects of different cluster geometries (linear, triangular, and more complex arrangements). By examining various configurations, we aim to provide a deeper understanding of how the interactions between spins in these clusters are governed by both the unique structural features of the fullerene molecules and their molecular levels. Our compuational study explores the role of spin exchange interactions, the potential for spin frustration, and how these phenomena can be manipulated to achieve desired magnetic behaviors, thus it can guide the design of new materials for spintronic devices, quantum information processing, and other applications where precise control over spin-spin interactions is key.

MA 45.2 Fri 9:45 H18

Intrinsic Spin Nernst Effect and Chiral Edge Modes in vdW Ferromagnetic Insulators: Dzyaloshinskii-Moriya vs. Kitaev Interactions — •Verena Brehm and Alireza Qaiumzadeh — NTNU Trondheim, Norway

The thermomagnetic Nernst effect and chiral edge states are key signatures of nontrivial topology and emerging Berry curvature in magnonic systems. Implementing atomistic spin simulations, we theoretically demonstrate the emergence of chiral magnon edge states at the boundaries of a ferromagnetic hexagonal lattice in the presence of Dzyaloshinskii-Moriya and Kitaev interactions, which are robust against nonlinear magnon interactions. In our simulations, we consider the spin parameters of CrI3 as a prototype of van der Waals magnetic layers. We show that the spin accumulation is reduced in the presence of Kitaev spin interactions compared to systems governed by Dzyaloshinskii-Moriya interactions. This reduction stems from the breaking of the U(1) symmetry, which leads to a shorter spin coherence length imposed by the Kitaev interaction. We propose that measuring the angular dependence of the Nernst signal in a magnetic field provides an effective indirect method for identifying the microscopic origin of topological magnons. Our findings hold promising potential for advancing next-generation energy-harvesting Nernst materials and facilitating the integration of topological magnetic materials with spintronic-based quantum technologies.

MA 45.3 Fri 10:00 H18

Origin of MAE and second order MAE due to the magnetostriction in tetragonal systems - FePt study — •Dominik Legut[1] and Pablo Nieves[2] — [1]IT4Innovations, VSB-TU Ostrava, Ostrava, Czechia — [2]University of Oviedo, Oviedo, Spain

The origin of magnetocrystalline anisotropic energy (MAE) guided by spin-orbit coupling in the $L1_0$-FePt alloy was analyzed and the correlations among MAE and magnetoelastic (magnetostriction) constants $b's(\lambda's)$ by means of the electronic structure eigenvalues (orbital energies) and eigenfunctions (orbital occupancies) were established[1]. Our numerical analysis includes the convolution of the projected wavefunction (density of states) of each orbital of the Fe and Pt sub-lattices into their orbital energies and its contribution to the MAE,$b's$, and $\lambda's$. However, this corresponds to the zero strain situation. For a zero stress (realistic conditions used in experiments) situtation a very small correction is found for the first anisotropy constant $\Delta K_1/K_1 = 0.07\%$, while a much more significant contribution is obtained for the second one $\Delta K_2/K_2 = 21.86\%$. General analysis of this effect for tetragonal crystals is provided, finding that ΔK_1 will be always positive for any stable phase with this symmetry[2].

References:
1. T. Das, P. Nieves, D. Legut, J. Phys. D: Appl. Phys. **58**, 035004 (2025)
2. D. Legut, P. Nieves, Solid State Sciences (accepted)

MA 45.4 Fri 10:15 H18

High-throughput workflow for predicting magnetic ground states — •Hao Wang and Hongbin Zhang — Technical University of Darmstadt, 64287 Darmstadt, Germany

Obtaining the correct magnetic ground state is crucial for understanding the nature of magnetism and serves as a foundation for engineering functional magnetic materials for interesting applications. In this work, we present a high-throughput computational workflow designed to accurately determine the exchange interaction J_{ij} matrices and other relevant parameters for a wide range of magnetic systems. Combining the four-state energy mapping method with the Green's function approach, we construct symmetrized Heisenberg Hamiltonians to model magnetic interactions. Furthermore, by integrating atomistic spin dynamics Vampire package, our framework enables the efficient prediction of magnetic ground states. This scalable workflow not only improves computational efficiency for complex magnetic materials but also provides a robust platform for exploring the fundamental properties of magnetic systems.

MA 45.5 Fri 10:30 H18

Semiclassical approach to the exchange interactions and spin waves in double-layered antiferromagnets — Seo-Jin Kim[1], Zdeněk Jirák[2], Jiří Hejtmánek[2], Karel Knížek[2], Helge Rosner[1], and •Kyo-Hoon Ahn[2] — [1]Max Planck Institute for Chemical Physics of Solids, D-01187 Dresden, Germany — [2]Institute of Physics, Czech Academy of Sciences, Cukrovarnická 10, 162 00 Praha 6, Czechia

We investigate the stability and magnonic properties of double-layered antiferromagnets using two model systems—the linear chain (LC) and a more complex railroad trestle (RT) geometry—as well as the real solid antiferromagnetic (AFM) CrN in its rock-salt structure. In the LC model, the spin-paired order ($\cdots ++ -- \cdots$) requires alternating ferromagnetic (FM) and AFM interactions. In contrast, the RT geometry allows some frustration, and the spin-paired order can be stable even for all magnetic exchange interactions being AFM. In the hypothetical cubic phase of CrN, magnetic Cr ions form a face-centered cubic lattice with equivalent AFM links to twelve nearest neighbors. However, the magnetostructural transition to an orthorhombically distorted phase below the Néel temperature ($T_N = 287$ K) diversifies the Cr-Cr nearest-neighbor distances, suppressing frustration. Using *ab initio* exchange parameters, we calculate the magnon dispersion relation and the temperature-dependent evolution of ordered magnetic moments. Our findings demonstrate that the stability of the double-layered AFM structure in CrN is attained, even when intra-sublattice interactions remain all AFM, consistent with the RT model.

MA 45.6 Fri 10:45 H18

Tuning Magnetic Anisotropy in Fe3Y Through Transition Metal Doping: An Ab-Initio High-Throughput Study — •Md Nur Hasan and Heike Herper — Department of Physics and Astronomy, Uppsala University, Box 516, SE-75120, Uppsala, Sweden

The advancement of permanent magnet systems is essential for various applications, including energy generation and information technology. This research focuses on developing and optimizing new permanent magnetic materials using an ab initio based first-principles approach. The Fe3Y system was initially selected for its in-plane magnetic anisotropy with a Curie temperature of 550 K, which, although advantageous, constrains its use in scenarios that require uniaxial (out-of-plane) anisotropy. The main goal of this study is to transition the magnetic anisotropy from the in-plane to a uniaxial configuration. Various transition metals were systematically introduced into both the Y and Fe sites of the Fe3Y structure to facilitate this shift. This doping approach enabled the tuning of the magnetic properties and provided insight into the mechanisms governing magnetic anisotropy. As a result, we identified several promising compositions with significant alterations in magnetic behavior, including systems that exhibit uniaxial anisotropy with Curie temperatures of ~ 550K, making them suitable for high-performance magnetic applications. Initial findings suggest that certain transition metal dopants can significantly modify spin-orbit coupling and crystal field effects, achieving the desired anisotropy realignment with the potential to discover a new category of high-performance permanent magnets.

15 min. break

MA 45.7 Fri 11:15 H18

Programmable Magnetophononics: Selective Damping of Surface Acoustic Waves — •Michael Karl Steinbauer[1], Peter Flauger[1], Bernhard Emhofer[1], Matthias Küss[2], Stephan Glamsch[2], Manfred Albrecht[2], and Claas Abert[1] — [1]University of Vienna — [2]University of Augsburg

Surface acoustic wave (SAW) bandpass filters are an indispensable part of modern telecommunications infrastructure [1]. Spin waves (SWs) can be excited by SAWs in radio-frequency bands, making their coupling a topic of current scientific interest [2].

In this work, we utilize this magnon-phonon interaction to demonstrate the theoretical viability of a novel device composed of exchange-decoupled magnetic islets on a piezoelectric substrate. Depending on the magnetic orientation of neighboring islets, a shift in the dispersion relation of the SW is predicted to occur due to their stray field interaction. This shift increases or decreases the efficiency with which the SAW can excite the SWs, leading to a difference in the amount of energy the magnetic system absorbs. For certain geometries, a gap in the SAW power after traversing the device of 10 dB/mm or more is predicted to occur.

For this study, a new algorithm for efficiently calculating SAW attenuation under the assumption of a continuous signal was developed for the micromagnetic simulation library magnum.np [3].

[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 45.8 Fri 11:30 H18

Mean-Field Approximation and ab-initio calculations in Tetragonal Mn_2-based Heusler compounds. — •Jorge Cardenas-Gamboa[1,5], Arthur Ernst[2], Maia G Vergniory[3,4], Edouard Lesne[1], Claudia Felser[1], and Paul McClarty[6] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]Johannes Kepler University of Linz, Linz, Austria. — [3]Donostia International Physics Center, Donostia-San Sebastian,Spain — [4]Université de Sherbrooke, Sherbrooke J1K 2R1 QC, Canada. — [5]Leibniz Institute for Solid State and Materials Research, Dresden, Germany — [6]Universite Paris-Saclay, Gif-sur-Yvette, France.

Achieving flexible control over magnetic properties is possible in multicomponent systems consisting of several magnetic sublattices with competing interactions.In 2014, Meshcheriakova et al. demonstrated that the Heusler compound Mn_2RhSn exhibits substantial strong non-collinearity and its magnetic structure undergoes a spin-reorientation transition, driven by the competition between its magnetic sublattices. In this work, we use a mean-field approximation to analyze the exchange interactions between the sublattices and investigate how different magnetic regimes develop as a function of temperature. Additionally, we perform first-principles calculations to derive the exchange interactions and assess their influence on the magnetic properties, extending our analysis to other tetragonal Heusler magnets. We then explore the topological properties that arise from the magnetism, focusing on the Weyl nodes and surface states.

MA 45.9 Fri 11:45 H18

First-Principles Study of Non-Collinear Magnets: Spin Models and Cluster Multipole Theory — •Juba Bouaziz[1,2], Takuya Nomoto[3], and Ryotaro Arita[1,2,4] — [1]RCAST, University of Tokyo, Japan — [2]CEMS, RIKEN (Wako), Japan — [3]Tokyo Metropolitan University, Japan — [4]Department of Physics, University of Tokyo, Japan

We present a computational approach for modeling complex non-collinear magnets using the cluster multipole (CMP) method [1] to determine symmetry-allowed magnetic configurations. The magnetic ground state is obtained by comparing the energies of candidate CMP solutions within a spin model Hamiltonian that includes isotropic exchange interactions, relativistic anisotropic terms, and higher-order biquadratic interactions. The parameters of the spin model are systematically calculated using the magnetic force theorem from the paramagnetic reference state [2]. This method is successfully applied to the TM3X Kagome magnet family (TM = Mn, Fe; X = Ga, Ge, Sn), demonstrating its computational efficiency and potential for high-throughput studies of unconventional non-collinear magnetic systems.

[1] M. T. Suzuki et al., Phys. Rev. B 95, 094406 (2017); [2] B. L. Gyorffy et al., J. Phys. F: Met. Phys. 15 1337 (1985).

MA 45.10 Fri 12:00 H18

Memory-Efficient Inverse Design for Advanced Magnonic Devices Using Level-Set Optimization — •Andrey Voronov[1,2], Marcos Cuervo Santos[2,3], Florian Bruckner[1,4], Dieter Suess[1,4], Andrii Chumak[1], and Claas Abert[1,4] — [1]Faculty of Physics, University of Vienna, Vienna, Austria — [2]Vienna Doctoral School in Physics, University of Vienna, Vienna, Austria — [3]Faculty of Sciences, University of Oviedo, Oviedo, Spain — [4]Research Platform MMM Mathematics - Magnetism - Materials, University of Vienna, Vienna, Austria

Inverse design in magnonics utilizes the wave nature of magnons and machine learning to develop logic devices with unique functionalities. However, existing methods face memory constraints, limiting the exploration of complex systems.

To address this, we integrate a level-set parameterization approach with an adjoint state method for memory-efficient simulations of magnetization dynamics. Implemented in neuralmag, a GPU-accelerated micromagnetic software, this framework enables efficient optimization of device topologies.

We validate the approach through two tasks: optimizing the shape of a magnetic nanoparticle to control hysteresis behavior and designing a 300-nm-wide yttrium iron garnet demultiplexer for frequency-selective spin-wave separation. These results showcase the algorithm's robustness and versatility in enabling the design of advanced magnonic devices for computational logic technologies.

MA 45.11 Fri 12:15 H18

Magnetoelectric coupling in type-I multiferroics via domain walls — •Aditya Putatunda and Sergey Artyukhin — Istituto Italiano di Tecnologia, Genova, Italy 16123

Type-I multiferroics, where ferroelectricity (FE) and magnetism arise independently with a large FE polarization but often tend to have a much weaker coupling to spins, e.g.: prototypical BiFeO3. Electric polarization, arising from inversion breaking, causes structural modifications across polarization domains in such materials. Here we demonstrate an effective coupling mechanism caused due to such structural modifications which in turn modifies the magnetic exchanges between the ions using first-principles density functional calculations. Magnetic domain walls, generally more mobile than polarization walls, depending on the nature of the materials, experience an effectively attractive or repulsive potential due to these modified exchanges. Such a potential can be taken advantage of in driving magnetic domain walls by sweeping polarization domains using electric field, thus giving rise to a cross-coupling mechanism, a highly sought phenomenon for novel low-power device applications.