MA 49: Focus Session: Higher-Order Magnetic Interactions – Implications in 2D and 3D Magnetism II

Time: Thursday 15:00–17:00 Location: HSZ 04

Invited Talk MA 49.1 Thu 15:00 HSZ 04

The role of itinerant electrons and higher order magnetic interactions among fluctuating local moments in producing complex magnetic phase diagrams. — Julie Staunton[1], Eduardo Mendive-Tapia[1,2], and •Christopher Patrick[1,3] — [1]University of Warwick, U.K — [2]Max-Planck Institut Fur Eisenforschung GmbH, Germany — [3]University of Oxford, U.K.

When external stimuli or varying temperature alter its magnetic properties a metal's complex electronic fluid with its emergent magnetic 'local moments' transforms. In this context the ab initio Density Functional Theory-based Disordered Local Moment method can successfully locate and characterise magnetic phase transitions and calculate caloric effects. It will be shown how the theory provides a Gibbs free energy function of local moment order parameters with two central objects - local moment correlation functions in the paramagnetic state and local internal magnetic fields as functions of magnetic order. The potentially most stable magnetic phases and dominant interactions between pairs of local moments are identifiable from the first. Higher order correlations extracted from the second produce effective 'multi-site' magnetic interactions depending on how the electronic structure evolves with the state and extent of magnetic order. The approach will be illustrated by applications to the magnetic order of the heavy rare earth metals, the tricritical metamagnetism in frustrated antiferromagnets with rich magnetic-strain phase diagrams and associated caloric effects, and finally the exceptional non-hysteretic first order magnetic phase transition in the divalent lanthanide compound Eu2In.

MA 49.2 Thu 15:30 HSZ 04

Origin of the short-period magnetic structure of MnGe from a first-principles high-temperature free energy — •Eduardo Mendive Tapia[1,2], Manuel dos Santos Dias[1], Stefan Blügel[1], and Samir Lounis[1] — [1]Peter Grünberg Institute and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany — [2]Department of Computational Materials Design, Max-Planck Institut für Eisenforschung, 40237 Düsseldorf, Germany

The helimagnetism of B20-type compounds such as MnSi and FeGe is usually understood as a competition between the ferromagnetic exchange interaction and the chiral Dzyaloshinskii-Moriya interaction. The magnetism of MnGe defies this interpretation owing to the short-period of its 3q magnetic structure and distinct B-T magnetic phase diagram [1]. Using a Disordered Local Moment theory implemented in the Korringa-Kohn-Rostoker method [2,3], we construct a first-principles high-temperature free energy for MnGe, which explains the short-period from competing long-range interactions. Our calculations also reproduce experimental volume-dependence of both the period and the Néel transition temperature. The first-principles magnetic phase diagram obtained points to the importance of higher-order magnetic exchange interactions to explain the observed 3q and 4q magnetic structures.—Work funded by the DAAD and EU Horizon 2020 via ERC-consolidator Grant No. 681405–DYNASORE.

[1] Fujishiro *et al.*, Nat. Commun. **10**, 1059 (2019)
[2] Gyorffy *et al.*, J. of Phys. F: Metal Phys. **15**, 1337 (1985)
[3] Jülich KKR codes (https://jukkr.fz-juelich.de)

MA 49.3 Thu 15:45 HSZ 04

Beyond Heisenberg exchange: non-collinear formalism for bcc Fe — •A. Szilva[1], D. Thonig[1], P.F. Bessarab[2,3], Y. O. Kvashnin[1], D. C. M. Rodrigues[1,4], R. Cardias[1,4], M. Pereiro[1], L. Nordström[1], A. Bergman[5,6], A. B. Klautau[4], and O. Eriksson[1,7] — [1]Department of Physics and Astronomy, Division of Materials Theory, Uppsala University, Box 516, SE-75120 Uppsala, Sweden — [2]Science Institute of the University of Iceland, 107 Reykjavik, Iceland — [3]Department of Nanophotonics and Metamaterials, ITMO University, 197101 St. Petersburg, Russia — [4]Faculdade de Física, Universidade Federal do Pará, Belém, 66075-110, Brazil — [5]Maison de la Simulation, USR 3441, CEA-CNRS-INRIA-Université Paris-Sud-Université de Versailles, F-91191 Gif-sur-Yvette, France — [6]INAC-MEM, CEA, F-38000 Grenoble, France — [7]School of Science and Technology, Örebro University, SE-701 82 Örebro, Sweden

The orbital resolved LKAG exchange calculations show that an entirely different microscopic mechanisms work in the T2g than in the Eg (and "mixed") orbitals in bcc Fe. Study of interatomic exchange parameters in a non-collinear framework, which parameters can be interpreted as higher order spin terms, too, is in line with these findings: the nearest-neighbor exchange parameters related to the T2g orbitals are essentially Heisenberg-like, ie., they do not depend on the underlying spin-configuration. In contrary, in the Eg and mixed channels strong configuration dependence can be found when one spin is fully rotated in a ferromagnetic background. The presentation is mostly based on the results published on Ref Phys. Rev. B 96 (14), 144413 (2017).

MA 49.4 Thu 16:00 HSZ 04

Short- and long-range toroidal order in nanomagnetic arrays — •Jannis Lehmann[1], Amadé Bortis[1], Naëmi Leo[2,3], Claire Donnelly[2], Peter Derlet[2], Laura J. Heyderman[1,2], and Manfred Fiebig[1] — [1]Department of Materials, ETH Zurich, Switzerland — [2]Paul Scherrer Institute, Villigen PSI, Switzerland — [3]CIC nanoGUNE, Donostia-San Sebastián, Spain

Ferrotoroidicity, i.e. the collective alignment of uniformly-oriented magnetic whirls that spontaneously form at the unit-cell level, is an elusive type of magnetically-compensated ferroic order. Since compounds displaying ferrotoroidicity are rare and difficult to identify because the access to their compensated magnetic order is experimentally challenging, we here make use of artificial planar nanostructures made from ferromagnetic building blocks as a versatile approach to design and study magnetic frustration or other phenomena. We introduce arrays of stray-field-coupled single-domain- or vortex-state nanomagnets of different geometry that exhibit emergent ferrotoroidic order at mesoscopic length scales. We perform magnetic force microscopy to achieve spatial access to the magnetic configuration and the toroidal domain pattern. By varying the arrangement of building blocks we tune the delicate competition of microscopic couplings between the nanomagnets. We find that this competition influences key observables of ferroic order as e.g. the domain size, the domain-wall configuration and the density of topological defects. We explain our observations by identifying different multipolar pathways to long-range order.

MA 49.5 Thu 16:15 HSZ 04

Competing Non-collinear Magnetic Phases in Osmates Double Perovskites — •Dario Fiore Mosca — University of Vienna & VDSP, Vienna, Austria

The interplay between electron correlation, local symmetry and spin-orbit coupling is among the most challenging aspect of condensed matter physics. These energy scales are simultaneously active in 5d transition metal oxides, which represent a rich playground for discovering new quantum states of matter. In particular, strong relativistic effects can lead to the formation of complex non-collinear magnetic orderings, whose origin cannot be understood within a standard Heisenberg picture. In our work, we study the ground state of the $5d^1$ osmate-based double perovskite Ba_2NaOsO_6 and decipher the driving mechanism that leads to the onset of the observed canted antiferromagntic pattern. The structural, electronic and magnetic properties of Ba_2NaOsO_6 are computed using fully relativistic and magnetically constrained DFT + U. We find that the magnetic energy landscape (in particular the canting angle) depends critically on the cooperative Jahn-Teller distortions and on the strength of the effective electron correlation U-J. In order to acquire additional information on the quantum origin of the canted AFM state we map the first principles total energies onto an extended pseudospin Hamiltonian, and find that dipolar and octupolar terms are the key interactions that drive the stabilization of the noncollinear ground state.

MA 49.6 Thu 16:30 HSZ 04

Hole doped 214-nickelate: A case study of spin dynamics in 3D-DCSS — •Rajesh Dutta[1,3] and Avishek Maity[2,3] — [1]Institut für Kristallographie, RWTH Aachen University — [2]Technical University of Munich, Germany — [3]Heinz Maier-Leibnitz Zentrum, FRM-II, Garching)

Inelastic neutron scattering study on the magnetic excitation in a stripe-ordered Pr2-xSrxNiO4 at 5K reveal that dynamics are manifested by order magnetic incommensurability as result of admixing 1/3-

stripe with the checkerboard matrix in NiO2 plane so called discommensurated spin stripe (DCSS). A suggested linear spin-wave model accounting 3D- DCSS with two-fold exchange interactions between Ni2+ spins, provides a good agreement with the measured spin wave dispersion up to 64 meV, notably, to describe a slight symmetric shift of the broadened peak in the energy range of 35 - 45 meV. Our results indicate that DCSS model is essential to consolidate in the LSWT calculation to understand the microscopic effect of doped holes on the spin microstructure.

MA 49.7 Thu 16:45 HSZ 04

Long-range chiral exchange interaction in synthetic antiferromagnets — Dong-Soo Han[1], Kyujoon Lee[1], •Fabian Kammerbauer[1], Myung-Hwa Jung[2], and Mathias Kläui[1] — [1]Institute of Physics, Johannes Gutenberg-Universität Mainz, Mainz, Germany — [2]Department of Physics, Sogang University, Seoul, Republic of Korea

The exchange interaction underlies all spintronic devices. This interaction has two counterparts * the symmetric and antisymmetric part. The symmetric term governs the ferro- and antiferromagnetism where the antisymmetric which has recently gained interest since it promotes topologically non-trivial chiral spin textures that promise new magnetic devices . So far, the antisymmetric exchange interaction has only been demonstrated in the rather short range limited to a single magnetic layer. Here we report a long-range antisymmetric interlayer exchange interaction in perpendicularly magnetized synthetic antiferromagnets with parallel and antiparallel magnetization alignments [1]. The measured asymmetric hysteresis loops under an in-plane field reveal a unidirectional and chiral nature of this interaction, resulting in canted magnetic structures. We explain our results by considering spin*orbit coupling combined with reduced symmetry in multilayers. Our discovery of a long-range chiral interaction provides an additional handle to engineer magnetic structures and could enable three-dimensional topological structures. [1] D.Han et al., Nature Mater. 18, 905 (2019)