MA 11: Computational Magnetism 1

Time: Monday 15:00–17:00 Location: H48

MA 11.1 Mon 15:00 H48

Monte Carlo modeling of magnetic crystals from graphical input — Michael Giger, •Amadé Bortis, Manfred Fiebig, and Thomas Lottermoser — Department of Materials, ETH Zurich

Magnetism in crystals can be described by a spin Hamiltonian which contains all the magnetic interactions between spins. The resulting magnetic properties of the material, like the spin-ordering or the critical behavior, can be derived from Monte Carlo simulations. The correct and efficient implementation of such a Hamiltonian into a computer program for the simulation is error-prone and time-consuming. Here, we present a tool where the magnetic interactions can be defined by connecting atoms in a three-dimensional visualization of a crystal. Our software then automatically generates an efficient code for the Monte Carlo simulations. All simulation parameters can be set in a graphical user interface. We will showcase our software by reproducing the magnetic order in the prototypical antiferromagnet Cr_2O_3 as an example. Our tool thus makes Monte Carlo simulations of complex spin systems more accessible to non-specialist users.

MA 11.2 Mon 15:15 H48

AiiDA-UppASD: Automatic workflow engine for high-throughput mag-netic simulations and machine learning — •Qichen Xu[1,2,3], Jonathan Chico[4], Manuel Pereiro[2], Danny Thonig[5], Erik Sjöqvist[2], Olle Eriksson[2], Anders Bergman[2], and Anna Delin[1,3] — [1]KTH Royal Institute of Technology, Stockholm,Sweden — [2]Uppsala University, Uppsala, Sweden — [3]Swedish e-Science Research Center, Stockholm,Sweden — [4]Sandvik Coromant, Stockholm, Sweden — [5]Örebro University,Örebro,Sweden

The ever-raising theoretical peak performance and accessibility of supercomputer resources bring automated simulations to a more important position for studies of magnetic materials properties. Recently, Huber et al. developed the AiiDA framework. In order to perform high-throughput atomic spin dynamics (ASD) simulations and take advantage of AiiDA platform and its build-in DFT plugins, we introduce the AiiDA-UppASD plugin which allows users to access to the majority of the functionalities of the UppASD code within the AiiDA framework via a Python package. In addition, several robust built-in workflows are also provided for managing ASD simulations, handling possible errors, and providing common modular workchains. With these workflows, complex tasks like high-throughput simulations of magnetodynamic properties as well as the determination of spin-wave excitation spectra and magnetic phase diagrams can be performed in a very efficient manner. Meanwhile, a machine learning (ML) prepared data generation workflow is also designed in order to offer ASD-related databases for the ML community to benchmark and develop methods.

MA 11.3 Mon 15:30 H48

Calculation of magnetic properties using Green's functions in the LAPW basis — •Henning Janssen[1,2], Stefan Blügel[1], Gustav Bihlmayer[1], and Alexander Shick[3] — [1]Forschungszentrum Jülich, Jülich, Germany — [2]RWTH, Aachen, Germany — [3]Czech Academy of Sciences, Prague, Czech Republic

Green's functions are a powerful tool for understanding responses and interactions, including the magnetic properties, in materials.

A method for calculating Green's functions utilizing the Kramers-Kronig transformation is presented. The implementation of this method in the linearized augmented plane-wave basis, as implemented in the Fleur code [1], is especially suited for orbitals mainly localized inside the Muffin-tin regions around the atoms. These Green's functions are used to calculate magnetic properties including the Heisenberg exchange constants J_{ij} or the Dzyaloshinskii-Moriya Interaction (DMI) using force-theorem methods [2] and non-collinear torques. Results for these calculations are shown for bulk systems of iron and Co/Pt films.

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[1]: www.flapw.de

[2]: A. I. Liechtenstein, et al. J. Magn. Magn. Mater. **67**, 65 (1987)

MA 11.4 Mon 15:45 H48

Ab initio study of exchange interactions at planar defects of crystal lattices — •Martin Zelený[1], Monika Všianská[2], Denis Ledue[3], Renaud Patte[3], Miroslav Černý[4], Ladislav Straka[5], and Oleg Heczko[5] — [1]Institute of Materials Science and Engineering, Faculty of Mechanical Engineering, Brno University of Technology, Brno, Czech Republic — [2]Department of Chemistry, Faculty of Science, Masaryk University, Brno, Czech Republic — [3]Normandie Université, UNIROUEN, INSA Rouen, CNRS, GPM, Saint Étienne du Rouvray, France — [4]Central European Institute of Technology, Brno University of Technology, Czech Republic — [5]FZU - Institute of Physics of the Czech Academy of Sciences, Czech Republic

Planar defects play an important role in crystalline magnetic materials, because they serve as obstacles to magnetic domain wall motion. Atomistic description of the magnetic properties requires knowledge of exchange interaction parameters J_{ij} between two atomic sites. These parameters can be found in literature for many bulk magnetic materials. However, very little is known about J_{ij} in the vicinity of planar defects where the symmetry of crystal lattice is reduced and atoms have different chemical environment. We provide deep analysis of J_{ij} obtained from ab initio calculations in the vicinity of the clean $\Sigma5(310)$ grain boundary in bcc Fe as well as grain boundary with segregated P impurities. We analyze also J_{ij} parameters in the vicinity of twin boundaries and antiphase boundaries in Ni_2MnGa magnetic shape memory alloys. Our results show strong influence of planar defects on exchange interactions.

MA 11.5 Mon 16:00 H48

Computationally Driven Evaluation of Magnetocrystalline Anisotropy — •Simone Köcher[1,2] and Stefano Sanvito[1] — [1]School of Physics / CRANN, Trinity College Dublin, Ireland — [2]IEK-9 - Fundamental Electrochemistry, Forschungszentrum Jülich, Germany

Custom-tailored magnetic materials are a crucial component in numerous modern technologies. The experimental search for new high-performance magnets can profit considerably from guidance by computational screening approaches, which however depend on reliable first-principle methods for calculating the key physical properties which underlie the magnetism of the material. One of them is the magnetocrystalline anisotropy (MCA), which contributes to the magnetic hardness.

For the well-studied $X(acac)_3$ (X = transition metal) coordination complexes we specifically explore and compare different methods for calculating the MCA: the finite energy difference approach (force theorem) within periodic boundary conditions and all-electron, full-potential perturbative approaches ranging from PT2 on PBE DFT to CASSCF-PT2 and NEVPT2. We explicitly study the influence of cluster geometry and various computational parameters at different levels of theory. Finally, we address the challenges involved in high-throughput MCA calculations for material screening applications.

MA 11.6 Mon 16:15 H48

Functional RG for Rydberg Array Spin Hamiltonians — •Benedikt Schneider — Physics Department, Arnold Sommerfeld Center for Theoretical Physics, and Center for NanoScience, Ludwig Maximilian University Munich, 80333, Germany

Rydberg-Atom arrays are a versatile platform to simulate strongly correlated phenomena from spin liquids to lattice gauge theories. We develop a functional renormalization group approach based on Kitaev's pseudo-Majorana spin representation that produces quantitative accurate results for Rydberg array Hamiltonians at finite temperature. A special feature of our approach is that implementation of infinite lattices with long-range interactions and complicated lattice geometries is straightforward.

MA 11.7 Mon 16:30 H48

Hubbard interactions in 2D magnetic $FePS_3$ and CrI_3 — •Fatemeh Haddadi[1], Edward Linscott[1], Marco Gibertini[2], Iurii Timrov[1], and Nicola Marzari[1] — [1]THEOS and MARVELL, EPFL, Lausanne, Switzerland — [2]University of Modena and Reggio Emilia, Modena, Italy

Hubbard-corrected density-functional theory has proven to be successful in addressing self-interaction errors in 3D magnetic materials. However, the effectiveness of this approach for magnetic 2D materials has remained elusive. Here, we use PBEsol+U and its extensions to inves-

tigate the electronic, structural, and vibrational properties of two 2D magnets: antiferromagnetic $FePS_3$ and ferromagnetic CrI_3. Hubbard parameters are computed from first-principles using density-functional perturbation theory (DFPT) [PRB 98, 085127 (2018)], thus avoiding any empiricism. First, we show that for $FePS_3$ the Hubbard corrections are crucial for obtaining the experimentally observed insulating state with the correct crystal symmetry. While empirical U can lead to instabilities, the Hubbard parameters from DFPT stabilize the ground state. We show that Hubbard-corrected vibrational frequencies are in good agreement with Raman experiments. Finally, we discuss 2D CrI_3, and the requirements it elicits in correcting separately the majority and minority bands.

MA 11.8 Mon 16:45 H48

Magnetism in strongly correlated twisted bilayers from first principles — •Aditya Putatunda and Sergey Artyukhin — Italian Institute of Technology, Genova, Italy

Twisted bilayer structures of van der Waals materials attract experimental and theoretical interest because of easy single layer exfoliation and processing and a variety of correlated states.1,2 Magnetic twisted bilayers hosting skyrmions have recently been demonstrated.3 Within first-principles approach, large supercells and tight convergence are required to compute magnetic interactions. Here we combine DFT and model simulations of Wannier function based tight-binding Hamiltonian to study the states in the twisted bilayer of CrI3.

[1] Xu et al., Nature Nanotechnology 17, 143*147 (2022) [2] N. Sivadas., Nano Lett. 18, 7658*7664 (2018) [3] Shang et al., ACS Appl. Nano Mater. 3, 1282*1288 (2020)