MA 1: Computational Magnetism I

Time: Monday 9:30–12:45 Location: HSZ 04

MA 1.1 Mon 9:30 HSZ 04

Accelerated evaluation of thermal conductivity via machine learning: A case study of two-dimensional (2D) BN — •Yixuan Zhang, Chen Shen, and Hongbin Zhang — Institute of Materials Science, TU Darmstadt, 64287 Darmstadt, Germany

Accurate density functional theory (DFT) calculations to evaluate the anharmonic effect are demanding, as accurate force constants from DFT up to the third or even higher orders are needed. In this work, using the recently developed machine learning technique, we obtained accurate force constants by learning over a limited number of configurations and demonstrated that the thermal conductivity can be evaluated accurately. The interatomic potential is developed using the GAP model, and the resulting forces are fed into Alamode to evaluate the thermal conductivity. The configurations for training were automatically selected using the active learning method, which enables future on-the-fly calculations. For 2D BN sheets, it is demonstrated that the final training set can be reduced to 123 out of total 867 geometries, and the resulting thermal conductivity is only slightly deviated from the values obtained via explicit DFT calculations. It is suspected that the method can be applied to other 2D/3D compounds where the computational effort required can be reduced by one order of magnitude.

MA 1.2 Mon 9:45 HSZ 04

High-throughput Screening for Novel MAB Phases — •Chen Shen, Qiang Gao, and Hongbin Zhang — Institute of Materials Science, TU Darmstadt, 64287 Darmstadt, Germany

The MAB phases are transition metal (M) borides with layered structures, which display a spectrum of intriguing magnetocaloric, mechanical and corrosion properties. In this work, based on density functional theory (DFT) calculations carried out in a high-throughput (HTP) way, we investigated systematically the stabilities and magnetic properties of six classes of MAB phases, e.g., MAB, M_2AB_2, $M_3A_2B_2$,M_3AB_4, M_4AB_4 and M_4AB_6, and three competitive phases such as M_5AB_2, $M_4A_3B_2$ and $M_3A_2B_2$, where M = Cr, Mn, Fe, Co and Ni; A = an arbitrary element from Li to Bi without inert gas and 4f rare-earth elements. Based on the thermodynamic phase diagram, it is predicted that there are tens of unreported MAB compounds which are stable. Moreover, it is found that several MAB compounds are promising permanent magnets with significant magnetocrystalline anisotropy (MAE) and sizable magnetization. For instance, the MAE of Mn_2PtB_2 is as large as 20.27 MJ/m^3. We believe such compounds are promising for future applications as functional magnetic materials.

MA 1.3 Mon 10:00 HSZ 04

Impact of the magnetic structure on the phase stability and functional properties of binary and ternary Mn alloys — •Ingo Opahle, Nuno Fortunato, Harish K. Singh, Qiang Gao, Oliver Gutfleisch, and Hongbin Zhang — Institute of Materials Science, TU Darmstadt, 64287 Darmstadt, Germany

Mn alloys are of interest for hard magnetic, magnetocaloric and spintronics applications. The magnetic structure of Mn alloys can be complex, which makes computational high-throughput predictions of novel Mn based functional materials highly demanding.

We use high-throughput density functional calculations to determine the magnetic ground state of known compounds in several binary and ternary Mn alloy systems. Initial spin structures are obtained by algorithms based on maximal magnetic subgroups and antiferromagnetic coupling of sublattices. We show that the magnetic structure can have a strong impact on the calculated phase stability. For binary alloys of Mn with Ir, Pt and Au the formation energy for the ground state is up to 250 meV/atom lower compared to calculations with an assumed ferromagnetic structure. Phase diagrams assuming a ferromagnetic structure are unreliable for these systems and can not be used to identify important magnetic materials like Mn_3Ir used in exchange biased films for data storage or the spin-orbit-torque compound Mn_2Au.

Based on the magnetic ground state phase diagrams we performed structure type searches and discuss potentially new stable binary phases. Further, the impact of the magnetic structure on functional properties of Mn alloys is illustrated at hand of a few examples.

MA 1.4 Mon 10:15 HSZ 04

Electric field control of magnetism without currents: from experiments to ab-initio spectroscopy calculations. — •Eszter Simon, Alberto Marmodoro, Sergey Mankovsky, and Hubert Ebert — Department Chemie, Ludwig-Maximilians-Universität München

Recent x-ray magnetic dichroism (XMCD) experiments [1-3] have shown that the magnetic properties of an ultra thin Pt layer can be controlled by application of an electric field across the interface with a ferromagnetic substrate and through an insulating layer that prevents actual charge transport. We discuss ab-initio investigations of this experimental setup by means of a simple extension of the Korringa-Kohn-Rostoker method [3]. Our all-electron, fully relativistic implementation of the 2D TB-KKR scheme for semi-infinite systems allows to gain insight into the role of different lattice terminations in connection with spin-orbit coupling effects, to evaluate the role of dielectric/capping layers, and to cross-compare out-of-equilibrium results due to the applied finite perturbation in terms of ground state properties and theoretical spectroscopy simulations.

[1] F.Matsukura et. al., Nat.Nanotech **10**, 209 (2015). [2] S.Miwa et al., Nat.Comm. **8**, 15848. (2017). [3] K. Yamada et al., Phys. Rev. Lett. **120**, 157203 (2018).

MA 1.5 Mon 10:30 HSZ 04

Electric field control of magnetism through transverse currents: first-principles calculations on XAS/XMCD experiments. — Sergey Mankovsky, •Alberto Marmodoro, Eszter Simon, and Hubert Ebert — Department Chemie, Ludwig-Maximilians-Universität München

Recent x-ray magnetic dichroism spectroscopy (XMCD) experiments have investigated a variety of electric field-controlled magnetism scenarios [1-3]. We consider a 2D Co/Pt heterostructure, studied in various geometries, under the influence of an applied electric field parallel to the interface and also to the equilibrium magnetization direction. This setup has been reported to produce an additional, perpendicular out-of-plane magnetization contribution, proportional to the current density and detectable through variation in the absorption cross-section for circularly polarized x-ray at the Co $L_{2,3}$ edges [3]. We investigate this effect by means of first-principles linear response calculations, performed at a fully relativistic level using the Korringa-Kohn-Rostoker method based on DFT. The scheme allows us to assess different physical mechanisms behind the experimental observation, to explore the impact of sample thickness and surface/interface effects, and study effects of spin-orbit torque, spin accumulation and to cross-compare ab-initio results with calculated XMCD spectra.

[1] R.Kukreja et al., PRL **115**, 096601 (2015). [2] K. T. Yamada et al., PRL **120**, 157203 (2018). [3] C.Stamm et al., PRB **100**, 024426 (2019).

MA 1.6 Mon 10:45 HSZ 04

Thermodynamics of the S=1/2 Pyrochlore Antiferromagnet — •Robin Schaefer, David Luitz, and Imre Hagymási — Max-Planck-Institut für Physik komplexer Systeme, Dresden, Germany

Studying three-dimensional frustrated quantum magnets is a challenging problem in general. Here we use several complementary techniques to study the high temperature behavior of the low spin pyrochlore quantum antiferromagnet: DMRG and quantum typicality yield exact results for small systems.
In order to test the stability of the features in the specific heat in the thermodynamic limit, we use the numerical linked cluster expansion, a systematic high temperature series expansion.
Rather than the usual approach based on clusters composed of single spins, we use physically motivated clusters of complete tetrahedra (i.e. complete unit cells), effectively allowing to access much higher orders of the expansion than otherwise possible. This combination of methods yields consistent results on the location of the high temperature peak of the specific heat.

15 min. break.

MA 1.7 Mon 11:15 HSZ 04

Robust first-principles scheme for extracting exchange interactions from full-potential electronic structure calculations — •Vladislav Borisov[1], Yaroslav O. Kvashnin[1], Pa-

trik Thunström[1], Anders Bergman[1], Anna Delin[3], Manuel Pereiro[1], Erik Sjöqvist[1], Danny Thonig[2], and Olle Eriksson[1,2] — [1]Department of Physics and Astronomy, Uppsala University, 75120 Uppsala, Sweden — [2]School of Science and Technology, Örebro University, 70182 Örebro, Sweden — [3]Department of Applied Physics, School of Engineering Sciences, KTH, Kista, Sweden

The design and optimization of magnetic materials can be done efficiently using first-principles electronic structure methods that allow to determine the microscopic mechanisms behind exchange interactions, which drive a particular magnetic behavior. The critical part of this approach is the mapping of the original electronic system onto a Heisenberg spin model. This requires the definition of a local projection for each magnetic atom, which may influence the calculated exchange interactions. In order to circumvent this problem, we propose a robust projection scheme within the RSPt full-potential electronic structure code for a reliable calculation of the magnetic exchange and demonstrate its performance for a few representative systems, including 3d and 4f metals, AFM insulators and low-dimensional systems. In the latter case, the inversion-symmetry breaking and spin-orbit coupling give rise to non-collinear magnetic textures, due to the Dzyaloshinskii-Moriya or higher-order interactions that can be analyzed using the proposed formalism.

MA 1.8 Mon 11:30 HSZ 04

Dzyaloshinskii-Moriya interaction enhanced reorientation in Fe_2W — •Balázs Nagyfalusi[1], László Udvardi[1,2], László Szunyogh[1,2], and Levente Rózsa[3] — [1]Department of Theoretical Physics, Budapest University of Technology and Economics, Budapest, Hungary — [2]MTA-BME Condensed Matter Research Group, Budapest University of Technology and Economics, Budapest, Hungary — [3]Universität Konstanz, Konstanz, Germany

The magnetic ground state of an Fe bilayer on W(110) substrate is a normal-to-plane alignment which on higher temperatures turns into the $(1\bar{1}0)$ in-plane direction. We investigated this phenomenon with metadynamics Monte Carlo simulations[1] based on a classical Heisenberg model, and found that the neglection the antisymmetric part of the exchange tensor, i.e. the Dzyaloshinskii-Moriya interaction the reorientation no longer occurs. The simulation has been performed using exchange tensors and anisotropy parameters obtained from ab-initio calculations.

1. B. Nagyfalusi *et al.* https://arxiv.org/abs/1907.03616

MA 1.9 Mon 11:45 HSZ 04

Ab-initio study of phase transitions in Fe100-xAlx alloys — •Vasily Buchelnikov, Mariya Matyunina, and Mikhail Zagrebin — Chelyabinsk State University, Chelyabinsk, Russia

Fe-Al-based functional materials are perspective for industrial application due to the unique combination of properties such as high strength, corrosion stability, low density, and low cost. It would be interesting to estimate structural and magnetic phase transition temperatures in the most questionable area of 10-40 at.% of Fe-Al with different structures. In this work, based on structural and magnetic phase transition temperatures estimated theoretically from the first principles, the concentration phase diagram for Fe100-xAlx ($15.625<x<31.25$ at.%) was plotted. Structural phase transition temperatures for the experimentally observed crystal structures were obtained from the structural optimization. It is shown that for x=28.125 at.% L12-like phase with slight distortions is energetically favorable. The ground state energy and magnetic moments of Fe75Al25 with different structures were calculated within GGA and GGA+U approaches. It is shown that in the case of GGA+U approximation, L12 phase becomes more stable compared with D03. The Curie temperatures were estimated from mean field approximation and Monte Carlo simulations using ab initio calculated exchange coupling constants. Both structural and magnetic phase transition temperatures are found in qualitative agreement with the experiment. Depending on Al concentration, five different sequences of phase transitions are observed in the phase diagram.

MA 1.10 Mon 12:00 HSZ 04

Variational Monte Carlo approach for the dynamical spectra of frustrated spin systems — •Francesco Ferrari[1,2] and Federico Becca[3] — [1]Institut für Theoretische Physik, Goethe-Universität Frankfurt, Frankfurt Am Main (Germany) — [2]SISSA-ISAS, International School for Advanced Studies, Trieste (Italy) — [3]Università degli Studi di Trieste, Trieste (Italy)

Inelastic neutron-scattering experiments provide fundamental insights into the behavior of magnetic systems and constitute the method of choice for the detection of the spin-liquid phase in candidate materials. However, the theoretical and numerical calculation of dynamical spectra, which are directly measured in neutron-scattering experiments, represents a formidable task in the context of frustrated magnetism. In our work, we employ an efficient variational Monte Carlo scheme to compute the spin dynamical structure factor of frustrated spin models.

We present our numerical results for the dynamical spectra of the antiferromagnetic J1-J2 Heisenberg model on the triangular lattice [1]. In the Heisenberg limit (J2=0), where the system is magnetically ordered, our variational spectra display a well-defined magnon branch, in contrast with spin-wave predictions of spontaneous magnon decay, and in agreement with recent DMRG calculations and inelastic neutron-scattering experiments on Ba3CoSb2O9. When frustration is included, the system undergoes a phase transition to a spin-liquid phase, whose spectral features indicate the presence of fractionalized spinon excitations, and highlight the important role played by gauge fluctuations.

[1] F. Ferrari and F. Becca, Phys. Rev. X 9, 031026 (2019).

MA 1.11 Mon 12:15 HSZ 04

Quantum effects in thermally activated domain wall switching in ferromagnets. — •Grzegorz Kwiatkowski[1] and Pavel F. Bessarab[1,2] — [1]University of Iceland, Reykjavík, Iceland — [2]Peter Grünberg Institute and Institute for Advanced Simulation, Forschungszentrum Jülich, Jülich, Germany

Most widely used data storage technologies are based on nanoscale magnetic structures [1]. In order to improve both memory retention and energy efficient writability one needs to increase stability of magnetic samples without changing the energy barrier. Therefore, it is vital to optimise the preexponential factor in the Arrhenius law, which requires one to properly study the effect of internal degrees of freedom on thermal switching pocesses [2,3]. We present analytic estimation of rate of escape for domain wall switching in 3D samples with focus on how results scale with internal parameters and sample size. Since minimum excitation energy for high frequency magnon modes is larger than average energy of thermal fluctuations, we employ Bose-Einstein statistics, which leads to nontrivial temperature dependencies of the preexponential factor. Our results open up new possibilities for enhancing stability of magnetic structures by entropic effects.

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[1] W. A. Challener et al. Nat. Photon. volume 3 (2009)
[2] P. F. Bessarab et al. Phys. Rev. Lett. 110.2 (2013)
[3] G. Fiedler et al. J. Appl. Phys. 111 (2012)

MA 1.12 Mon 12:30 HSZ 04

Dynamical structure factors of dynamical quantum simulators — •Maria Laura Baez[1,2], Marcel Goihl[2], Jonas Haferkamp[2], Juan Bermejo-Vega[2,3], Marek Gluza[2], and Jens Eisert[2,4] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Dahlem Center for Complex Quantum Systems, Berlin, Germany — [3]Institute for Theoretical and Computational Physics, Granada, Spain — [4]Helmholtz-Zentrum Berlin für Materialen und Energie, Germany

The dynamical structure factor is one of the experimental quantities crucial in scrutinizing the validity of the microscopic description of strongly correlated systems. Despite its long-standing importance, it is exceedingly difficult in generic cases to numerically calculate it, ensuring that the necessary approximations involved yield a correct result. We discuss in what way results on the hardness of classically tracking time evolution under local Hamiltonians are precisely inherited by dynamical structure factors; and hence offer in the same way the potential computational capabilities as dynamical quantum simulators do. Furthermore, we improve upon a novel, readily available, measurement setup allowing for the determination of the dynamical structure factor in different architectures, including arrays of ultra-cold atoms, trapped ions, Rydberg atoms, and superconducting qubits. Our results suggest that quantum simulations employing near-term quantum devices allow for the observation of dynamical structure factors of correlated quantum matter in the presence of experimental imperfections, for larger system sizes than what is achievable by classical simulation.