MA 42: Magnetic Heuslers

Time: Friday 11:30–12:45 Location: H48

MA 42.1 Fri 11:30 H48

First-principles study of magnetic tunnel junctions based on half-metallic and spin-gapless semiconducting Heusler compounds: Reconfigurable diode and inverse TMR effect — •Thorsten Aull, Ersoy Sasioglu, and Ingrid Mertig — Martin-Luther-Universität Halle-Wittenberg, Institut für Physik, 06120 Halle (Saale)

Magnetic tunnel junctions (MTJs) based on half-metallic magnets (HMMs) and spin-gapless semiconductors (SGSs) exhibit unique properties, such as current rectification, i.e., diode effect, and reconfigurability in addition to a tunnel magnetoresistance (TMR) effect [1]. We investigate from first-principles MTJs based on SGS and HMM quaternary Heusler compounds [2]. Our quantum transport calculations have demonstrated that these MTJs exhibit current rectification with high on/off ratios. Moreover, depending on the relative orientation of the magnetization of the electrodes, the MTJ allows the electrical current to pass either in one or the other direction, which leads to an inverse TMR effect. We show that, in contrast to conventional semiconductor diodes, the rectification bias voltage window of the MTJs is limited by the spin gap of the HMM and SGS Heusler compounds. The combination of nonvolatility, reconfigurable diode functionality, and high Curie temperatures of the electrode materials makes the proposed MTJs very promising for room temperature spintronic applications and opens new ways to magnetic memory and logic concepts.

[1] N. Maji and T. Nath, Appl. Phys. Lett. **120**, 072401 (2022).
[2] T. Aull *et al.*, arXiv:2202.06752 (2022).

MA 42.2 Fri 11:45 H48

Exploring all 3d-metal Heusler alloys for functional properties: density functional theory + Monte Carlo study — •Madhura Marathe and Heike C. Herper — Department of Physics and Astronomy, Uppsala University, 75120 Uppsala, Sweden.

The search for cost-effective and rare-earth metal free permanent magnets is essential for various applications. In this study, we explore a novel class of Heusler alloys consisting of all 3d-metals. We do high-throughput studies using an electronic structure database to search for X_2YZ-type Heuslers (X = Fe, Ni) with tetragonal symmetry and high magnetic moments. We perform density functional theory calculations to obtain the ground state structure, magnetic anisotropy energy (MAE) as well as the exchange interaction parameters J_{ij} for selected materials. Using the calculated J_{ij}'s, we map our system on a Heisenberg model and perform Monte Carlo simulations to calculate the Curie temperature. Through such multiscale modeling, we aim to identify potential candidates for permanent magnets. We find that for these systems J_{ij}'s have oscillations over a long range with both ferromagnetic and antiferromagnetic interactions, and it is essential to include these in the model to capture correct transition.

MA 42.3 Fri 12:00 H48

High-throughput calculations on Co-based Heusler alloys assisted with the measurement of phase diagram in the related ternary system — •Kun Hu — Technical University Darmstadt Otto-Berndt-Straße 3, 64287 Darmstadt

Abstract: High-throughput (HTP) density functional theory (DFT) calculations have been carried out on Co-based Heusler alloys, combined with Exact Muffin-Tin Orbitals (EMTO) methods and Uppsala Atomistic Spin Dynamics (UppASD) package. Firstly, the stability of the Co2XY and X2CoY phases have been calculated and selected as parent phases which mainly center on the crystal structure and the tetragonal distortion considering formation energy and distance to the convex hull. And then, the specific properties of curie temperature (Tc) and magneto-crystalline anisotropy energy (MAE) of these phases have been calculated, of which some typical compounds show a high Tc and large MAE. Furthermore, the phase diagram of Co-Pt-Ti, Co-Ge-Ti, Co-Ge-Zr, and Co-Ge-Hf ternary systems were measured through a technique of alloy sampling and diffusion triple. Based on the results from Electron Probe Microanalysis (EPMA) and X-ray diffraction (XRD) techniques, the isothermal sections of these systems were constructed at different temperatures. Several ternary phases were detected and the relevant composition range was confirmed. The current study found interesting results that the Heusler phase Co2TiGe showed a remarkable composition range.

MA 42.4 Fri 12:15 H48

Tuning of the effective magnetic decoupling in Ni-Mn-(In,Sn) Heusler alloys — •Olga N. Miroshkina[1], Francesco Cugini[2,3], Simone Chicco[2], Fabio Orlandi[4], Giuseppe Allodi[2], Pietro Bonfà[2], Vincenzo Vezzoni[2], Lara Righi[2,3], Franca Albertini[3], Roberto De Renzi[2], Massimo Solzi[2,3], and Markus E. Gruner[1] — [1]Department of Physics and CENIDE, University of Duisburg-Essen, Duisburg, Germany — [2]University of Parma, Parma, Italy — [3]IMEM-CNR, Parma, Italy — [4]Rutherford Appleton Laboratory, Chilton, Didcot, Oxfordshire, United Kingdom

The magnetocaloric effect at first-order phase transitions is considered as an efficient and ecologically friendly alternative to conventional compressor cooling. This contribution is devoted to the complex magnetic ordering mechanisms in magnetocaloric Ni-Mn-(In,Sn) Heusler alloys, which we explore by means of density functional theory. The calculations accompany extensive experimental investigations, which reveal a non-monotonic trend in the Curie temperature and an effective magnetic decoupling of 4a and 4b sublattices [1]. Our first-principles calculations confirm a composition-dependent competition of the effective ferromagnetic and antiferromagnetic coupling between the sublattices, which can be directly controlled by electron doping in terms of In/Sn substitution. This result shows the possibility of fine-tuning of Heusler materials via exchanging the main-group element increasing the range of their potential applications. This work is funded by DFG within CRC/TRR 270 (project no. 405553726).

[1] F. Cugini et al., Phys. Rev. B 105, 174434 (2022).

MA 42.5 Fri 12:30 H48

Noncollinear magnetic order in epitaxial thin films of the MnPtGa hard magnet — •Rebeca Ibarra[1,2], Edouard Lesne[1], Bachir Ouladdiaf[3], Ketty Beauvois[3], Alexandr Sukhanov[2], Rafal Wawrzyńczak[1], Walter Schnelle[1], Anton Devishvili[3], Dmytro Inosov[2], Claudia Felser[1], and Anastasios Markou[1] — [1]Max-Planck-Institute für Chemische Physik fester Stoffe, D-01187 Dresden, Germany — [2]Institut für Festkörper- und Materialphysik, Technische Universität Dresden, D-01069 Dresden, Germany — [3]Institut Laue-Langevin, CS20156, 38042 Grenoble Cedex 9, France

Noncollinear magnetism has attracted great attention in the recent years and promise rich exotic properties with potential for spintronic applications. In this work, we present a detailed analysis of the structural and magnetic properties of high-quality thin films of the hexagonal MnPtGa hard magnet grown on $Al_2O_3(0001)$ substrates. The films crystalize in the $P6_3/mmc$ space group, with an ordering temperature of $T_C = 263$ K into a ferromagnetic (FM) state, followed by a spin reorientation transition at $T_{sr} \sim 160$ K. A large uniaxial magnetic anisotropy is observed in this centrosymmetric compound. We further investigate the magnetic transitions by single-crystal neutron diffraction at zero applied magnetic field. The emergence of the structurally forbidden (001) Bragg reflection for $T < 160$ K, unequivocally determines a transition to a spin canted state, where the Mn magnetic moments align ferromagnetically along the c-axis and antiferromagnetically in the basal plane, resulting in a spin canting angle of 20° respect to the c-axis.