MM 55: Computational Materials Modelling - Magnetic Materials

Time: Thursday 11:45–13:00 Location: IFW B

MM 55.1 Thu 11:45 IFW B

A Phase Field Crystal Model for Magneto-Structural Interaction — •Rainer Backofen[1] and Axel Voigt[1,2] — [1]Institute of Scientific Computing, Technische Universität Dresden, 01062 Dresden, Germany — [2]Dresden Center for Computational Materials Science (DCMS), 01062 Dresden, Germany

Phase field crystal (PFC) modeling is based on a free energy for a smoothed particle density. The energy is minimized by a smoothed particle density, that has the basic symmetry of the crystal. Thus, defects, elasticity and plasticity is natural included.

In order to include magneto-structural interaction, local magnetization is coupled with a structural PFC model [1,2]. We will discuss the coupling and show how to control the magnetic properties of the model. This extended PFC model is used to study the impact of external magnetic fields on grain boundary movement and on coarsening in thin films [2].

[1] N.Faghihi et al. PRE 88, 032407 (2013).

[2] R. Backofen et al. PRL 122, 126103 (2019).

MM 55.2 Thu 12:00 IFW B

Modeling of magnetodyanmics in endohedral-fullerene-based molecular magnets — •Stanislav Avdosheno and Alexey Popov — Leibniz Institute for Solid State and Materials Research (IFW), D-01069 Dresden, Germany

Systems dynamics is the merit of the system complexity. In the single molecular magnets(SMMs) research, there are many aspects that make SMMs very complex. Well before any magnetic measurements begin, the molecular dynamics control the structures and order of SMMs in bulks or on surfaces. In the end, this impacts strongly the magnetic feedback of the whole system. Through the magnetic measurement itself, the magnetic states evolve accordingly to the quantum equation of motion. The quantum dynamic is coupled strongly with local atomic motions with substantial effects on magnetic stability.

In this contribution, we report such dynamical effects in the application to the endohedral-fullerene-based molecular magnets. We showed how the molecular dynamics modeling helps to understand which structural elements to expect on the metallic and dielectric surfaces. Having used ab initio methods, we have been able to derive the fundamental properties of Ln containing endohedral-fullerene molecular magnets. This helped to rationalize and to have a deep understanding of magnetic relaxation in these systems. Finally, we also introduced a simple model, based on the existing open quantum systems theories, able to predict the spin relaxation dynamics with implicit and explicit phonons in the system Hamiltonian.

MM 55.3 Thu 12:15 IFW B

An advanced method for computing the intrinsic spin Hall conductivity from first principles — •Minsu Ghim, Ji Hoon Ryoo, and Cheol-Hwan Park — Department of Physics and Astronomy, Seoul National University, Seoul 08826, Korea, Center for Correlated Electron Systems, Institute for Basic Science, Seoul 08826, Korea, Center for Theoretical Physics, Seoul National University, Seoul 08826, Korea

Spin Hall effect plays a key role in spintronics. It is widely accepted that the spin Hall conductivity can be categorized into three different contributions: skew-scattering, side-jump, and intrinsic. Recently, methods for computing the intrinsic spin Hall conductivity from first principles using the maximally-localized Wannier functions have been reported [1,2]. In this talk, we present technical improvements of the original method [2] in terms of computational efficiency.

[1] J. Qiao, J. Zhou, Z. Yuan, and W. Zhao, Phys. Rev. B 98, 214402 (2018) [2] J.-H. Ryoo, C.-H. Park, and I. Souza, Phys. Rev. B 99, 235113 (2019)

MM 55.4 Thu 12:30 IFW B

A three-order-parameter, bistable, magnetoelectric multiferroic metal — Andrea Urru[1,2], Francesco Ricci[3], Alessio Filippetti[1], Jorge Iniguez[4], and •Vincenzo Fiorentini[1] — [1]Dip Fisica, Uni Cagliari, Italy — [2]SISSA, Trieste, Italy — [3]University of Louvain-la-neuve, Belgium — [4]LIST, Luxembourg

Using first-principles calculations we predict that the layered-perovskite metal Bi5Mn5O17 is a ferromagnet, a (switchable) ferroelectric, and a ferrotoroid, and has two energy-degenerate ground states with distinct polar, magnetic, and toroidic axes. In both states, the three vector order parameters (polarization, magnetization, ferrotoroidic moment) are mutually orthogonal, so they can be rotated globally by switching between ground states. Importantly, Bi5Mn5O17 is expected to be thermodynamically stable in O-rich growth conditions.

MM 55.5 Thu 12:45 IFW B

Magnetic and Electronic properties of Mn2Au: A Novel spintronic compound — •Sunil Wilfred DSouza[1], Hans-Joachim Elmers[2], Satya Prakash Bommanaboyena[2], Martin Jourdan[2], and Jan Minár[1] — [1]New Technologies Research Centre, University of West Bohemia, Univerzitní 8, CZ-306 14 Pilsen, Czech Republic. — [2]Institut für Physik, Johannes Gutenberg-Universität, Staudingerweg 7, D-55099 Mainz, Germany

The band structure of bulk Mn2Au has been investigated by first-principles density-functional theory calculations based on the Green*s function technique. The total density of state reveals contributions mainly from the Au5d and Mn3d states with rigid local moments on the Mn sites. The existence of significant out-of-plane magnetic anisotropy combined with the large strength of short range antiferromagnetic exchange interactions between Mn atoms located at two different Wyckoff positions results in the stabilization of the antiferromagnetic ground state. Two dimensional plots of constant energy surfaces in the Γ-X-Σ plane of the Brillouin zone exhibits a four-fold to two-fold symmetry breaking as a function of the binding energy at 0.00 eV and 0.25 eV below the Fermi surface. We find that such a symmetry breaking in Mn2Au is arising due to the degeneration of the electronic bands in the presence of external magnetic field indicating a strong spin-orbit coupling interaction. Our results describes the tuning of the magnetic and electronic properties of Mn2Au for spintronic applications.