MM 16: Computational Materials Modelling - Novel Materials

Time: Monday 15:45–16:45 Location: IFW B

MM 16.1 Mon 15:45 IFW B

Ab initio derived phase stabilities for the design of novel Ce-based hard-magnetic materials — •Halil ibrahim Sözen, Fritz Körmann, Tilmann Hickel, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany

Due to the developments in electrical transportation and renewable energies, hard magnetic materials composed of rare earths (RE) and transition metals (TM) have gained increasing importance in the last decades. Recently, there are attempts to develop alternative hard magnetic materials, RE-TM-X (X=Ti, W, Mo, Si, Al), that lift the dependence on a small number of RE elements. In order to support the efforts to find alternative materials concepts for hard magnetic applications, we performed ab initio calculations of finite temperature phase stabilities of Ce-based alloys. The Helmholtz free energy F(T,V) is calculated for all relevant competing phases using a sophisticated set of methods capturing vibrational, electronic, magnetic and configurational entropy contributions. The study includes unary Ce, binaries of Ce-Fe and Fe-Ti phases, and ternary Ce-Fe-Ti phases, for which the performance of our approach for rare-earth metals is tested. We observe that the presence of the CeFe2 phase retards any formation of promising Ce-Fe-Ti alloys. The study has therefore been extended to the impact of fourth alloying elements such as Cu and La, in order to provide strategies to solve this challenge.

MM 16.2 Mon 16:00 IFW B

Possible Gating on the Surface of a Weak Topological Insulator: Bi14Rh3I9 — •Madhav Prasad Ghimire[1] and Manuel Richter[1,2] — [1]Leibniz Institute for Solid State and Materials Research, IFW Dresden, P.O. Box 270116, D-01171 Dresden, Germany — [2]Dresden Center for Computational Materials Science, DCMS, TU Dresden,D-01069 Dresden, Germany

Recently synthesized Bi14Rh3I9 was predicted to be a weak topological insulator. Scanning tunneling microscopy confirms this with a signatures of one-dimensional conducting states in the band gap at step edges of [(Bi4Rh)3I]2+ (2DTI) surface layers. However, the surface-layer gap is found 0.25 eV below the Fermi level (EF). Transport experiments are expected to be biased by intrinsic n-doping at the surface. Using density functional theory slab calculations we resolve this issue to shift EF into the surface layer gap without losing its topological properties. We perform chemical modification on the surface of Bi14Rh3I9: sparse layer of Iodine atoms is added onto the 2DTI surface. Investigation shows that deposition of one I atom per surface unit cell onto 2DTI surface opens a surface gap of 0.1 eV at EF, if simultaneously one I atom is removed from the dorsal spacer layer. The same effect with reduced gap size (0.08 eV) is observed for adding/removing I atoms in two fold higher concentration. Comparing our results with the experiment [ACS Nano, 2016] we predict that Fermi level can be shifted to the surface gap by deposition of I atoms onto the 2DTI surface in an appropriate range of concentration.

MM 16.3 Mon 16:15 IFW B

High Throughput searching for new topological materials — •Zeying Zhang[1,2], Yugui Yao[2], and Hongbin Zhang[1] — [1]Institute of Materials Science, TU Darmstadt, 64287 Darmstadt, Germany — [2]Beijing Key Laboratory of Nanophotonics and Ultrafine Optoelectronic Systems, School of Physics, Beijing Institute of Technology, Beijing 100081, China

The bottleneck of current studies on topological insulators is to identify better materials which can be fabricated into devices more feasibly. To search for novel topological materials, we developed a high throughput framework which can be utilized to screen over compounds with known crystal structures. We have applied our methods to ternary compounds of Bi and nitrides, with crystal structures obtained from Materials Project. For the moment, we focus on systems with small band gaps and with time-reversal symmetry. To characterize the topological properties including the surface states and topological invariants, the Wannier functions are constructed in an automated manner using a {\it poor-man's} algorithm, where the partial density of state from the first principles calculations is integrated in order to determine the proper projections and the energy windows. For the materials with inversion symmetry, we can easily get the topological invariants by counting the number of occupied states with odd parities. Till now, we have found two new topological compounds, and will discuss their topological properties in detail.

MM 16.4 Mon 16:30 IFW B

Charge transport in organic semiconductors: Towards an ACKS2-based polarizable force field — •Patrick Gütlein[1], Lucas Lang[1], Karsten Reuter[1], Jochen Blumberger[1,2], and Harald Oberhofer[1] — [1]Technische Universität München, Germany — [2]University College London, UK

Charge carrier transport, an integral part of diverse reactions and devices, is generally subject to the response of the surrounding environment. Especially in organic semiconductors the accurate theoretical treatment of the electronic rearrangements in the medium is a complex task. The high anisotropy and comparatively low dielectric screening require system sizes that challenge even efficient first-principles approaches like density-functional theory (DFT). In this situation the recently proposed atom-condensed Kohn-Sham density functional theory approximated to second order (ACKS2) approach[1] could represent a computationally undemanding, yet accurate alternative. In this approach, the linear response of the electron density and Kohn-Sham potential are captured by an atom-centered series expansion up to second order. For a range of molecular model systems we systematically compute the ACKS2 parameters with DFT and analyze their dependence on the intra-molecular degrees of freedom. We show that parts of the ACKS2 response can be approximated analytically, with the remaining parameters not varying strongly with respect to molecular motion. This represents an important first step in making ACKS2 applicable as a polarizable force field. [1] T. Verstraelen *et al.*, J. Chem. Phys. **138**, 7 (2013); *ibid* **141**, 19 (2014).