MM 33: Topical Session Electron Theory IV

Time: Thursday 11:00–13:00 Location: IFW A

Topical Talk MM 33.1 Thu 11:00 IFW A

Playground magnetism in low-dimensions: impact of first-principles theory — •Stefan Blügel — Peter Grünberg Institut & Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Metals in reduced dimensions developed to a playground for interesting magnetic phenomena. In low dimensions, metals that are nonmagnetic in bulk can become magnetic in low dimension, magnetic interaction strengths are largely modified and magnetic anisotropies change by orders of magnitude. Nanostructures with lattices of increasing topological frustration can be grown leading to magnetic structure of unprecedented complexity. Magnetic structures can be modified by local probes. The choice of the substrate is an additional parameter that can modify the physics of these systems. In this presentation is shown, how systematic first-principles calculations based on the density functional theory carried out with innovative cutting edge electronic structure methods can unravel the physical trends in the high-dimensional phase space of low-dimensional magnets and how that inspires suggestions of new systems with unexpected physical phenomena.

Topical Talk MM 33.2 Thu 11:30 IFW A

Metallic and half-metallic magnetism — •Jürgen Kübler — Technische Universität, Darmstadt, Germany

The topic of the talk is introduced by means of two (rather old) examples, RhMn3 and Mn3Sn; these are metallic magnets that order in different non-collinear moment arrangements. Density functional theory explains their peculiar ground states and allows a determination of the exchange interactions that result in fairly good estimates of their ordering temperatures. Work by Fähnle et al. on a fast approach to the simulation of spin dynamics is extended to Heusler compounds, for which the half-metallic gap is discussed together with examples of spin-wave spectra and the role of spin-orbit coupling. Some variants of tetragonal Heusler compounds are discussed that have magnetic properties which make them interesting for spintronics applications.

Topical Talk MM 33.3 Thu 12:00 IFW A

Strain effects in magnetic and ferroelectric complex oxides from first principles — •Claude Ederer — School of Physics, Trinity College, Dublin 2, Ireland

For many applications complex functional oxides are epitaxially grown on substrates with slightly mismatched lattice constants. The resulting epitaxial strain can have drastic effects on the functional properties of the thin film materials, and in fact provides an attractive way to optimize ferroic properties or stabilize new phases. First principles electronic structure calculations are a powerful tool to investigate these effects, and also allow to separate genuine strain effects from other influences that are generally present in thin film samples.

In this talk I will discuss several examples of strain effects in complex oxides and I will present results of first principles calculations that allow to clarify the underlying mechanisms. In particular I will discuss the recently observed strain-induced morphotropic phase boundary in multiferroic $BiFeO_3$, the occurrence of strain-induced ferroelectric instabilities in the magnetic perovskites $CaMnO_3$ and $LaCrO_3$, and the effect of epitaxial strain on the magneto-crystalline anisotropy in the spinel ferrites $CoFe_2O_4$ and $NiFe_2O_4$.

MM 33.4 Thu 12:30 IFW A

Order and phase stability in CoPt: the role of magnetism. — •Sondes Karoui[1], Hakim Amara[1], François Ducastelle[1], and Bernard Legrand[2] — [1]LEM, ONERA-CNRS, BP72 92322 Châtillon Cedex, France — [2]SRMP, CEA, Saclay, France

Transition metal nano-alloys (FePd, CoRh, and CoPt) are innovative new materials whose size and chemical composition govern their physical and chemical properties. CoPt, the focus point of this study, had been duly studied in the bulk phase both experimentally and theoretically. There exists a large array of results that clearly hint at the importance of magnetism, and the stabilization that it brings to the system. Indeed, we strongly believe that the crystallographic order present in CoPt can be attributed to the alloy*s inherent magnetic character.

To point out this effect, Density Functional Theory calculations have been performed using the ABINIT code with and without magnetism. We report on the influence of spin polarized calculations on structure stabilization in bulk Co and Pt as well as the alloy*s various crystallographic phases: ordered L1o, L12, and disordered FCC. This approach corresponds to a quantitative first step towards better understanding the role of magnetism at the atomic scale.

Reference 1 (submitted): S. Karoui, H. Amara, F. Ducastelle, and B. Legrand, First principle study of order and magnetism in Co(1-x)Pt(x).

MM 33.5 Thu 12:45 IFW A

Finite temperature magnetism combining first-principles and spin Quantum Monte Carlo — •Fritz Körmann, Alexey Dick, Tilmann Hickel, and Jörg Neugebauer — Max-Planck-Institut Düsseldorf, Max-Planck-Straße 1, 40074 Düsseldorf

The free energy of a system is a fundamental quantity for predicting phase diagrams, finite temperature materials parameters, or kinetic barriers. An ab initio derivation of it makes a highly accurate evaluation of all excitation processes mandatory. One of the most challenging - but for many engineering materials crucial - contributions arises from the magnetic degrees of freedom. We have developed a mapping procedure that transforms the full magnetic Hamiltonian onto an effective nearest-neighbor spin Hamiltonian. The latter can be directly solved employing spin quantum Monte Carlo calculations. We demonstrate the high accuracy achievable by the new approach by computing magnetic heat capacities and free energies for the magnetic pure elements Fe, Co, and Ni, and by extending it to magnetic compounds such as Cementite (Fe3C) [1]. In all cases, an excellent agreement with experimental data is found.

[1] Hallstedt, Djurovic, von Appen, Dronskowski, Dick, Körmann, Hickel, Neugebauer, Calphad 34, 129 (2010).