MM 23: Computational Materials Modelling: Magnetic & Electrical Properties

Time: Wednesday 15:45–18:30 Location: H44

MM 23.1 Wed 15:45 H44

Electronic structure of the non-centrosymmetric antiferromagnetic delafossite $AgCrSe_2$ — •Seo-Jin Kim[1], Haijing Zhang[1], Marcus Schmidt[1], Michael Baenitz[1], Gesa Siemann[2], Chiara Bigi[2], Phil D. C. King[2], and Helge Rosner[1] — [1]Max Planck Institute for Chemical Physics of Solids, D-01187 Dresden, Germany — [2]School of Physics and Astronomy, University of St. Andrews, St. Andrews KY16 9SS, United Kingdom

We present the theoretical studies of the electronic structure and the anomalous Hall effect in $AgCrSe_2$ based on density functional theory together with experimental results. $AgCrSe_2$ is a layered triangular lattice system that lacks inversion symmetry, and exhibits a ferromagnetic coupling in layer and an antiferromagnetic coupling between Cr adjacent layers. The comparison of the Cr partial DOS determined from the photoemission measurements and the magnetic LDA+U calculations with a value of U = 0.75 eV shows a good agreement, revealing that this compound is weakly correlated due to a strong hybridization with the ligands. The Se 4p states are dominating near the Fermi energy, resulting the sizable band split of the order of 300 meV induced by the SOC. Our recent work demonstrates that this system shows an unconventional anomalous Hall effect driven by the Rashba-like spin-orbit coupling due to the non-centrosymmetric structure. The anomalous Hall conductivity was calculated based on the Berry curvature using an effective tight-binding model constructed by the Wannier function approach. The calculated σ_{xy} shows a good agreement to the experimental measurement.

MM 23.2 Wed 16:00 H44

Atomistic simulations of electrocaloric effects in ferroelectric-paraelectric superlattices — •Diana Elisa Murillo Navarro[1,2], Hugo Imanol Aramberri Del Vigo[1], and Jorge Íñiguez[1,2] — [1]Materials Research and Technology Department, Luxembourg Institute of Science and Technology, Luxembourg — [2]Department of Physics and Materials Science, University of Luxembourg

Electrocaloric effects (i.e., the temperature change caused by the application or removal of an electric field) in ferroelectric materials could provide us with an alternative to current polluting cooling technologies. Ferroelecric/paraelectric superlattices, such as the PbTiO3/SrTiO3 system, usually present partly-disordered phases of high entropy (e.g., the so-called domain liquid state1) whose polarization can be condensed (frozen) under the application of an electric field, potentially triggering a large change in temperature. Here we present our latest theoretical results on such electrocaloric effects obtained from second principles simulations2.

Work funded by the Luxembourg National Research Fund through project C18/MS/12705883 *REFOX*.

1 P. Zubko et al., Nature 534, 524 (2016).

2 J.C. Wojdel et al., J. Phys.: Condens. Matt. 25, 305401 (2013).

MM 23.3 Wed 16:15 H44

Magnetically-textured superconductivity in elemental Rhenium — Gabor Csire[1], James F Annett[2], •Jorge Quintanilla[3], and Balazs Újfalussy[4] — [1]ICN2, Barcelona, Spain — [2]University of Bristol, Bristol, United Kingdom — [3]University of Kent, Canterbury, United Kingdom — [4]Wigner Research Centre for Physics, Budapest, Hungary

Recent μSR measurements revealed remarkable signatures of spontaneous magnetism coexisting with superconductivity in elemental rhenium. Here we provide a quantitative theory that uncovers the nature of the superconducting instability by incorporating every details of the electronic structure together with spin-orbit coupling and multi-orbital physics. We show that conventional s-wave superconductivity combined with strong spin-orbit coupling is inducing even-parity odd-orbital spin triplet Cooper pairs, and in presence of a screw axis Cooper pairs* migration between the induced equal-spin triplet component leads to an exotic magnetic state.

MM 23.4 Wed 16:30 H44

Magnetic bond-order potential for iron-cobalt alloys — •Aleksei Egorov, Aparna Subramanyam, Ralf Drautz, and Thomas Hammerschmidt — ICAMS, Ruhr-Universität Bochum, Bochum, Germany

We present a general-purpose analytic bond-order potential for large-scale simulations of magnetic FeCo alloys. The model is based on a *d*-valent orthogonal tight-binding Hamiltonian in two-center approximation and an embedding term to account for the s electrons. The BOP is a physical model and therefore requires only a comparably small set of reference data and only a small number of parameters to be optimized. It still provides good transferability to properties of FeCo that we did not include in the fit. We demonstrate the transferability of the FeCo BOP for defect formation energies, vibrational properties, and elastic constants. Due to the explicit treatment of magnetism, our BOP can reproduce the main features of the electronic structure of magnetic and nonmagnetic phases. The predictive power of the FeCo BOP yields a reasonable estimate of the order-disorder transition temperature of magnetic B2-FeCo. Our FeCo BOP also reproduces the dense sequence of stable structures for Fe-rich FeCo compounds.

MM 23.5 Wed 16:45 H44

Ab-initio High-Throughput Screening for Magnetic MAX Phases — •Ali Muhammad Malik, Jochen Rohrer, and Karsten Albe — Materials Modelling, Technical University of Darmstadt, Germany

MAX phases are layered ternary transition metal carbides and nitrides that combine both metallic and ceramic properties such as high toughness and strength at elevated temperatures. So far about ~80 single-M containing MAX phases have been synthesised. But very few of these phases, have long-range magnetic order and are mostly based on Cr and/or Mn. It is expected that magnetically ordered MAX phases will be promising in spintronics and magnetocaloric applications. In this work, we systematically search for stable MAX phases with a focus on magnetic properties, by screening about 1200 potential compositions. The thermodynamic stability is based on relative formation enthalpy compared to known competing phases that are present in M-A-X ternary phase diagram obtained from online databases e.g. Materials Project. Based on the evaluation of relative formation enthalpy, we have predicted around ~170 new MAX phases that are potentially synthesisable. However, out of these predicted phases, only 2 in total, based on Cr or Mn, were found to have long-range magnetic order. Finally, it is concluded that the incorporation of a late-transition metal into the MAX structure by alloying or unconventional post-synthesis routes, is the way forward for achieving magnetic long-range order.

15 min. break

MM 23.6 Wed 17:15 H44

Energetic and electronic properties of CsK_2Sb surface facets: An *ab initio* study — •Richard Schier[1,2], Holger-Dietrich Sassnick[2], and Caterina Cocchi[2,1] — [1]Humboldt-Universität zu Berlin and IRIS Adlershof — [2]Carl von Ossietzky Universität Oldenburg

For the efficient generation of ultra-bright electron beams, the microscopic understanding of the electronic structure of the photoemitting materials is crucial. Ternary alkali antimonides have been proposed as a promising class of photocathodes [1-4]. However, still little is known about their surface properties. We fill this gap with an ab initio study of the energetic and electronic properties of 7 CsK_2Sb surface facets of low Miller index. We investigate formation energies as a function of chemical potential to quantify the stability of these systems at varying concentration of the atomic species. We find that the (111)-surfaces terminated with K on top of Sb are generally the most stable, except for very high (low) concentrations of Cs (K). Calculated values for the work functions range from 2.33 eV for (100)-surfaces to 3.50 eV for (111)-surfaces terminated with a Sb layer. From the analysis of the band structures we find 4 out of 7 surfaces to be semiconducting. Metallic surfaces are formed upon an excess of metal atoms at the interface with vacuum.

[1] Schmeißer et al., PRAB 21, 113401 (2018). [2] Cocchi et al., JPCM 31, 014002 (2019). [3] Cocchi et al., Sci. Rep. 9, 18276 (2019). [4] Amador & Cocchi, JPCM 33, 365502 (2021).

MM 23.7 Wed 17:30 H44

Modeling Temperature-Dependent Electronic Structure of Semiconductors with a Dynamic Tight-Binding Approach —

•Martin Schwade, Maximilian Schilcher, and David Egger — Department of Physics, Technical University of Munich, Garching, Germany

For theoretical calculations of large-scale system sizes or longer time-scale phenomena the computational costs of typical density functional theory can present a steep barrier, which needs to be tackled by development of alternative approaches. Here, we propose an extension of the tight-binding (TB) formalism which allows for the calculation of macroscopic and temperature-dependent properties of semiconductors with little computational effort. In contrast to previous formulations, we fit TB parameters to first-principles energy eigenvalues using machine learning techniques. Furthermore, our TB approach employs hybrid orbital basis functions and addresses the problem of distance-dependent matrix elements by numerical integration of these orbitals. With this, we can maintain the average symmetry of the system as best as possible but still account for dynamic changes to that symmetry, e.g., by lattice distortions and other thermal effects. Our method is particularly helpful for getting an accurate solution of the electronic-structure problem for semiconductors at finite temperatures.

MM 23.8 Wed 17:45 H44

Coupled electronic and lattice degrees of freedom in excitonic insulator candidate Ta2NiSe5 and Ta2NiS5 — •Banhi Chatterjee, Jernej Mravlje, and Denis Golež — Jozef Stefan Institute, Jamova 39, SI 1000, Ljubljana, Slovenia

The origin of phase-transition from a high temperature orthorhombic phase to a low temperature monoclinic phase in Ta2NiSe5 is debatable. There are two competing scenarios, namely, a structural instability with a B2g zone center optical phonon and electronic order parameter of excitonic nature breaking the discrete set of lattice symmetries [1-3]. We defined a theoretical description which takes both scenarios on equal footings based on realistic modeling using DFT as a starting point and describe electronic and lattice correlation on a Hartree Fock level. We have identified both excitonic instability and the B2g phonon mode in our calculations and investigate the effect of electron-phonon coupling. Within our methods we have further identified spectroscopic signatures showing the lack of excitonic ordering in the auxiliary compound Ta2NiS5 which is in agreement with the experimental ARPES observations [4].

[1] A. Subedi, Phys. Rev. Mater. 4, 083601 (2020). [2] L. Windgätter, M. Rösner, G. Mazza, H. Hübener, A. Georges, A. J. Millis, S. Latini, and A. Rubio, Angel,npj Comp. Mat 7, 14 (2021) [3] G. Mazza, M. Rösner, L. Windgätter, S. Latini, H. Hübener, A.J. Millis, A. Rubio, and A. Georges, Phys. Rev. Lett. 124, 197601 (2020) [4] K. Mu, H. Chen, Y. Li, Y. Zhang, P. Wang, B. Zhang, Y. Liu, G. Zhang, Li. Song, and Z. Sun, J.of Mat. Chem. C. 6, 3981 (2018)

MM 23.9 Wed 18:00 H44

Supermetal-insulator transition in a non-Hermitian network model — •Hui Liu[1], Jhih-Shih You[2], Shinsei Ryu[3], and Ion Cosma Fulga[1] — [1]IFW Dresden and Würzburg-Dresden Cluster of Excellence ct.qmat, Helmholtzstrasse 20, 01069 Dresden, Germany — [2]Department of Physics, National Taiwan Normal University, Taipei 11677, Taiwan — [3]Department of Physics, Princeton University, Princeton, New Jersey, 08540, USA

We study a non-Hermitian and non-unitary version of the two-dimensional Chalker-Coddington network model with balanced gain and loss. This model belongs to the class $D^\dagger$ with particle-hole symmetry† and hosts both the non-Hermitian skin effect as well as exceptional points. By calculating its two-terminal transmission, we find a novel contact effect induced by the skin effect, which results in a non-quantized transmission for chiral edge states. In addition, the model exhibits an insulator to "supermetal" transition, across which the transmission changes from exponentially decaying with system size to exponentially growing with system size. In the clean system, the critical point separating insulator from supermetal is characterized by a non-Hermitian Dirac point that produces a quantized critical transmission of 4, instead of the value of 1 expected in Hermitian systems. This change in critical transmission is a consequence of the balanced gain and loss. When adding disorder to the system, we find a critical exponent for the divergence of the localization length $\nu = 1$, which is the same as that characterizing the universality class of two-dimensional Hermitian systems in class D.

MM 23.10 Wed 18:15 H44

Dynamical mean-field theory on the high-temperature superconductivity for cerium hydrides under extreme pressure — •Yao Wei and Cedric Weber — King's College London, London, UK

Hydrogen-rich superhydrides are promising high-Tcsuperconductors, with superconductivity experimentally observed near room temperature, as shown in recently discovered lanthanide superhy- drides at very high pressures, e.g. LaH10 at 170 GPa and CeH9 at 150 GPa. Superconductivity is believed to be closely related with the high vibrational modes of the bound hydrogen ions. Here we study the limit of extreme pressures (from 200 to 500 GPa or higher) where lanthanide hydrides with large hydrogen content have been observed. We focus on CeH10, the prototype candidate for achieving a large electronic contribution from hydrogen in the electron-phonon coupling. In this work, we use a first-principles calculation platform with the inclusion of many-body corrections to evaluate the detailed physical properties of the Ce-H system and to understand the structure, stability and superconductivity of these systems at ultra-high pressure. We provide a DMFT approach to further investigate conventional superconductivity in hydrogen rich superhydrides.