MM 38: Methods in Computational Materials Modelling (methodological aspects, numerics)

Sessions: Unconventional materials; Complex alloys and microstructure

Time: Thursday 15:00–17:30 Location: H44

MM 38.1 Thu 15:00 H44

Materials with helical architecture obtained by High Pressure Torsion Extrusion — •Roman Kulagin[1], Yan Beygelzimer[1,2], Yuri Estrin[3,4], Yulia Ivanisenko[1], Dayan Nugmanov[1], Andrej Mazilkin[1,5], and Horst Hahn[1] — [1]Institute of Nanotechnology, Karlsruhe Institute of Technology, Eggenstein-Leopoldshafen, Germany — [2]Donetsk Institute for Physics and Engineering named after A.A. Galkin, National Academy of Sciences of Ukraine, Kyiv, Ukraine — [3]Department of Materials Science and Engineering, Monash University, Clayton, Australia — [4]Department of Mechanical Engineering, The University of Western Australia, Crawley, Australia — [5]Institute of Solid State Physics, Russian Academy of Sciences, Chernogolovka, Russia

Composite materials are widely used in engineering. Commonly, reinforcements have simple shapes of granules, fibers or laminae. By using free-end torsion, one can transform straight fibers into helicoidal ones. The report describes the High Pressure Torsion Extrusion (HPTE) process, which allows performing more complex transformations. For example, straight fibers can be transformed to complex helicoidal surfaces. This greatly expands the range of achievable architectures of composites, while at the same time improving the strength of their constituents through extreme grain refinement. A simple analytical model developed in this work and verified experimentally provides a platform for design of composite materials with HPTE-induced inner architectures.

MM 38.2 Thu 15:15 H44

The Effect of the Hydrostatic Pressure on the Topology of the Electronic Charge Density of YbB_6 — •Niloofar Hadaeghi[1,2], Javad Nematollahi[1], Saeid Jalali Asadabadi[1], and Hongbin Zhang[2] — [1]Department of Physics, Faculty of Sciences, University of Isfahan, Isfahan, Iran — [2]Institute of Materials Science, Technische Universität Darmstadt, Darmstadt, Germany

Several rare-earth based hexaborides have been proposed to be strongly correlated topological Kondo insulators. In this work, the topology of the electronic charge density (TECD) for YbB_6 compound and its changes at finite pressure is investigated using density functional theory and quantum theory of the atoms in molecules, to search for possible transition in the topology of charge densities. The calculations were performed using the WIEN2k and CRITIC2 codes, within the GGA+U (U=7 eV) approximation with spin-orbit coupling. It is observed that no topological transition occurs in the charge density of YbB_6 when applying pressure, and no quasi-atom exists. Detailed analysis on the number of various types of critical points has been carried out, and the Morse relation is satisfied at both zero and finite pressures.

MM 38.3 Thu 15:30 H44

On the negative differential conductance of single-wall carbon nanotubes from ab-initio quantum simulations — •Jaime Silva[1], Bruce F. Milne[1,2], and Fernando Nogueira[1] — [1]CFisUC, Department of Physics, University of Coimbra, Rua Larga, 3004-516 Coimbra, Portugal — [2]Nano-Bio Spectroscopy Group, University of the Basque Country (UPV-EHU), Centro Joxe Mari Korta, Avenida de Tolosa, 72, 20018 Donostia-San Sebastian, Spain

Negative differential conductivity (NDC) is a current decrease when the voltage across certain materials is increased. It is important for oscillators, amplifiers, and fast switching devices. In this work, using real time quantum simulations, we show that this phenomenon occurs in isolated finite armchair single wall carbon nanotubes (SWCNT) without end contacts. For metallic SWCNT, like the armchair SWCNT, NDC due to electron transfer to secondary valleys is not expected to be observed, as a consequence of the two quantum channels at the Fermi energy that are available to conduction. The NDC is due to the finite nature of the SWCNT and the existence of excited states that are blocked, similarly to a Coulomb blockade system, thus preventing any further current flow. We also show that the SWCNT conductivity depends on its length and that the current flowing on the SWCNT behaves like a Bloch oscillation that is disrupted in the presence of a molecule, decreasing the conductivity, which explains the behaviour of SWCNT organic gas sensors.

MM 38.4 Thu 15:45 H44

Exchange-driven dimerization, magnetism and insulating state in diamond(111) — betul pamuk[1] and •matteo calandra[2] — [1]School of Applied and Engineering Physics, Cornell University, Ithaca, NY 14853, USA — [2]Sorbonne Université, CNRS, Institut des Nanosciences de Paris, UMR7588, F-75252, Paris, France

Strong electron-electron interaction in ultraflat edge states can be responsible for correlated phases of matter, such as magnetism, charge density wave or superconductivity. Here we consider the diamond(111) surface that after Pandey reconstruction, presents zig-zag carbon chains, generating a very flat surface band. By performing full structural optimization with hybrid functionals, we find that a substantial dimerization (0.076 Å bond disproportionation in the HSE06, 0.09 Å in PBE0) occurs on the chains; a structural effect absent in calculations based on the LDA/GGA functionals. This dimerization is the primary mechanism for the opening of an insulating gap. Neglecting spin polarization, the single-particle direct gap is 1.672 in PBE0 (1.0 in HSE06), smaller than the experimental data that are compatible with a $1.57-1.87$ (including $0.1-0.4$ eV of excitonic effects). However, the exchange interaction stabilizes a ferrimagnetic order along the Pandey π-chains with magnetic moments as large as $0.285\ \mu_B$, opening a direct band gap of approximately 2.1 eV in PBE0, in agreement with experiments. Our work is relevant for systems with flat bands in general and wherever the interplay between structural and electronic degrees of freedom is crucial, as in twisted bilayer graphene, IVB atoms on IVB(111) surfaces such as Pb/Si(111) or molecular crystals.

MM 38.5 Thu 16:00 H44

Unconventional superconductivity in a doped quantum spin Hall insulator — xianxin wu, mario fink, werner hanke, ronny thomale, and •domenico di sante — Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Am Hubland Campus Süd, Würzburg 97074, Germany

A monolayer of jacutingaite (Pt_2HgSe_3) has recently been identified as a novel quantum spin Hall insulator. By first-principles calculations, we study its Fermiology in the doped regime and unveil a type-I and type-II van Hove singularity for hole and electron doping, respectively. We find that the common link between the propensity for a topological band gap at pristine filling and unconventional superconductivity at finite doping roots in the longer ranged hybridization integrals on the honeycomb lattice. In a combined effort of random phase approximation and functional renormalization group, we find chiral d-wave order for the type-I and odd-parity f-wave order for the type-II regime.

MM 38.6 Thu 16:15 H44

Designing new two-dimensional Janus nanomaterials by anionic exchange — •Woosun Jang[1,2] and Aloysius Soon[1] — [1]Department of Materials Science & Engineering, Yonsei University, Seoul 03722, Korea — [2]Department of Inorganic Chemistry, Fritz-Haber-Institute of the Max-Planck-Society, Berlin 14195, Germany

Two-dimensional nanomaterials have played a key role in the recent advances in nanoscience for a decade, especially in the area of energy technology. Of late, a new class of 2D material has been suggested and experimentally realized – namely, the Janus monolayer. Different from preceding 2D materials, such as graphene and transition metal dichalcogenides, Janus monolayers lack the inversion symmetry in both in-plane and out-of-plane directions, and this leads to new anisotropic physiochemical properties which can be potentially useful for key energy applications. In this work, we design and investigate various novel two-dimensional Janus materials, via the anionic exchange method. In particular, by starting from the well-known MoS_2 and WS_2 monolayers, we substitute the top and bottom sulfur layers using a combination of group V and VII anions. Density-functional theory calculations are then performed to examine their anisotropic material properties.

15 min. break

MM 38.7 Thu 16:45 H44

Shandite Co3Sn2S2 - story and news — •Richard Weihrich — University of Augsburg, Regensburg, Germany

Shandite type compounds turned into focus with recent discoveries on Sn2Co3S2 = Co3Sn2S2 i.e. giant anomalous hall effects and magnetic Weyl semi metal characteristics. The compound was first synthesized and characterized in Regensburg in 1979 by Zabel and Range. After 2 decades the half metal ferromagnetism of highly anisotropic Sn2Co3S2 was discovered by DFT calculations in Regensburg, too. The story of the compound, discoveries and new results are reported and discussed.

MM 38.8 Thu 17:00 H44

Atomistic simulations of mixed 1/2 [111] dislocations in bcc transition metals — •Tapaswani Pradhan[1], Anastasiia Kholtobina[2], Lorenz Romaner[3], Matous Mrovec[4], and Ralf Drautz[5] — [1]Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Ruhr-Universität Bochum, Bochum, Germany — [2]Materials Center Leoben Forschungs GmbH, Leoben, Austria — [3]MCL Forschungs GmbH, Leoben, Austria — [4]ICAMS, RUB, Bochum, Germany — [5]ICAMS, RUB, Bochum, Germany

Structure and mobility of dislocations govern the mechanical properties of metals. It is widely accepted that in body-centered cubic (BCC) metals plastic deformation at low temperature is largely controlled by non-planar 1/2<111> screw dislocations. However, recently mixed 1/2<111> dislocations, which are predominantly of edge character and therefore expected to be glissile, were proposed to possess an unexpectedly high Peierls stress. In this study we investigate the core structures and mobilities of mixed 1/2<111> dislocations in five BCC transition elements Nb, Ta, Mo, W and Fe using atomistic simulations. The simulations were carried out with different models of interatomic interactions, ranging from classical potentials via tight-binding-based bond order potentials to first-principles methods based on density functional theory. Our study shows that both the predicted core structures and the Peierls barriers depend sensitively on the employed model and boundary conditions. We present a detailed comparison of different models and discuss the relation between atomic-scale properties and macroscopic behavior.

MM 38.9 Thu 17:15 H44

Simulation of Capillary-Driven Kinetics with Multi-Phase-Field and Lattice-Boltzmann — •Raphael Schiedung[1], Marvin Tegler[1], Dmitry Medvedev[2], and Fathollah Varnik[1] — [1]Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Ruhr-University Bochum, Bochum, Germany — [2]Lavrentyev Institute of Hydrodynamics SB RAS, Lavrentyev prosp. 15, 630090, Novosibirsk, Russia

We propose a combined computational approach based on the multi-phase-field and the lattice Boltzmann method for the motion of solid particles under the action of capillary forces. The accuracy of the method is analyzed by comparison with the analytical solutions for the force and motion of two parallel plates of finite extension connected by a capillary bridge. The method is then used to investigate the dynamics of multiple spherical solid bodies connected via capillary bridges. The amount of liquid connecting the spheres is varied, and the influence of the resulting liquid-morphology on their dynamics is investigated. It is shown that the method is suitable for a study of liquid-phase sintering which includes both phase transformation and capillary driven rigid body motion [1]. Furthermore, the combination with the multi-phase-field offeres the possibility to include effects relevant to solid-phase sintering [2, 3].