

MM 18: Computational Materials Modelling - Phase Stability I

Time: Tuesday 10:15–11:30

Location: H24

MM 18.1 Tue 10:15 H24

Stability and superconductivity of Ca-B under pressure — ●SHEENA SHAH¹ and ALEKSEY KOLMOGOROV² — ¹University of Oxford, UK — ²Binghamton University - SUNY, USA

In the search for MgB₂-like phonon-mediated superconductors, we have carried out a systematic DFT-based evolutionary crystal structure search of the whole Ca_xB_{1-x} system at gigapascal pressures. A set of diverse ground state boron structures are identified for CaB, CaB₂, CaB₄ and CaB₆. The monoboride is predicted to be superconducting at 5 K. Others are predicted to be superconducting at lower temperatures, demonstrating the inverse correlation between thermodynamic stability and superconducting properties. Finally, structural rules have been established for the thermodynamic stability of these alkaline earth metal borides with pressure. For example, we show that ThB₄-type CaB₄ is stable at ambient pressure since the ionic radius of Ca²⁺ is an ideal fit for the boron network.

MM 18.2 Tue 10:30 H24

A joint DFT and experimental study of the competing phases of Calcium at high-pressures and low-temperatures — ●DEEPA KASINATHAN¹, CARINA BOERRNERT¹, MICHAEL HANFLAND², JENS HUNGER¹, HELGE ROSNER¹, and ULRICH SCHWARZ¹ — ¹MPI CPFS-Dresden — ²ESRF, Grenoble

One of the most unanticipated developments in superconducting critical temperatures (T_c) in the past decade has been the achievement of much higher values of T_c in elemental superconductors by the application of high pressure. Surprisingly, these superconducting states evolve from simple metals that are non-superconducting at ambient pressure. Calcium undergoes a series of structural changes under pressure and superconducts with a T_c as high as 26 K near 160 GPa. There has been a long standing discrepancy among and between various experiments and as well as density functional theory based calculations to correctly identify the various high-pressure phases in calcium. Here, we report on a combined experimental and theoretical work on the multitude of structural phase transitions observed at low-temperatures and high-pressures. In our study, we have performed high-pressure X-ray diffraction experiments at the ESRF synchrotron beam-line (ID09A) to examine, verify and validate the complex phase diagram of calcium.

MM 18.3 Tue 10:45 H24

Crystal structure prediction and electronic properties of Li-based ternary compounds — ●MAIA G. VERGNIORY¹, MIGUEL A. L. MARQUES², SILVANA BOTTI², MAX AMSLER³, STEFAN GOEDECKER³, IRAIS VALENCIA², ANTONIO SANNA¹, EVGUENI V. CHULKOV⁴, ARTHUR ERNST¹, ALDO H. ROMERO¹, and EBERHARD K. U. GROSS¹ — ¹Max Planck Institute of Microstructure Physics, 06120 Halle, Germany — ²Universite de Lyon, F-69000 Lyon, France and LPMCN, CNRS, UMR 5586, Universite Lyon 1, F-69622 Villeurbanne, France — ³Department of Physics, Universitaet Basel, Klingelbergstr. 82, 4056 Basel, Switzerland — ⁴Donostia International Physics Center, 20018 Donostia-San Sebastian, Spain

On the basis of ab initio first principles and using the Minimal Hop-

ping Algorithm we predict the crystal structure of non synthesized LiYZ (Y=Au,Ag, Z=Te,Se) based ternary compounds. We find that, as distinct from expectation, the crystal structure depends strongly on the composition, thus every compound belongs to a different symmetry group and has complexly different electronic properties. We will analyze the fundamental physics below these features considering the calculated ground state structure.

MM 18.4 Tue 11:00 H24

The effect of partial occupancies on lithium ion diffusivity in lithium titanate oxides — ●BENEDIKT ZIEBARTH — IAM, Karlsruhe Institute of Technology, Kaiserstrasse 12, 76131 Karlsruhe, Germany — Fraunhofer Institute for Mechanics of Materials IWM, Wöhlerstrasse 11, 79108 Freiburg, Germany

The effect of partial occupancies on lithium ion diffusivity in lithium titanate oxides Lithium titanate oxide (LTO) is a promising candidate as an anode material in future generations of lithium ion batteries. In this work, we investigate the diffusion barriers for lithium ions in two different crystal structures of LTO using the density functional theory. Our calculations show that the activation barriers vary between 0.30–0.48 eV for the spinel phase Li₄Ti₅O₁₂ and between 0.20–0.51 eV in the lithiated rock salt phase Li₇Ti₅O₁₂. The origins of the rather broad ranges of activation energies are related to different chemical environments of the diffusion channels due to partial occupancies of some sites in LTO. Our results reveal that determination of lithium diffusion constants in LTO cannot be carried out by using a single activation barrier. Instead, the local chemical environment of the diffusion paths must be considered to correctly capture the variety of activation barriers.

MM 18.5 Tue 11:15 H24

Prediction of a hybrid graphene-diamond like phase — ●SILVIA BAHMANN, TORSTEN WEISSBACH, and JENS KORTUS — TU Bergakademie Freiberg, Institute of Theoretical Physics, D-09596 Freiberg, Germany

The crystal structure contains the most important information about a crystalline solid. Therefore, predicting it from first principles by just specifying the chemical composition has been long pursued. Increasing computer power in the last decade made it possible to explore the huge search space (3N + 3 dimensions where N is the number of atoms) of unknown crystal structures using density functional theory.

We applied an evolutionary strategy that uses the main features of natural evolution namely recombination, mutation, selection and the survival of the fittest and found a new hybrid graphene-diamond like phase. Our structure can be described as crossing graphene sheets that form nearly rectangular tubular pores. The atoms at the crossing lines show nearly perfect tetrahedral coordination whereas the ones in between exhibit sp³ bonding. Crossed graphene is shown to be dynamically stable with respect to phonons and elastic constants. The latter also point out the close relation to graphite/graphene. By inspecting the electronic structure similarities to graphene also become visible.