MM 25: Electronic properties II

Time: Wednesday 14:45–16:15 　　　　　　　　　　　　　　　　　　　　　　　　Location: H6

MM 25.1　Wed 14:45　H6

Valence-dependent Analytic Bond-order Potential for Transition Metals — •RALF DRAUTZ and DAVID PETTIFOR — Department of Materials, Unversity of Oxford, Oxford, UK

An analytic interatomic bond-order potential (BOP) is presented that depends explicitly on the valence of the transition metal element [1]. This analytic potential predicts not only the structural trend from hcp to bcc to hcp to fcc that is observed across the non-magnetic 4d and 5d transition metal series, but also the different ferromagnetic moments of the alpha (bcc), gamma (fcc) and epsilon (hcp) phase of the 3d transition metal iron as well as the difference between the ferromagnetic and anti-ferromagnetic states. In addition, this new potential includes a correct description of alloy bonding within its remit. In this talk we discuss how the potential is derived from the tight-binding electronic structure and demonstrate that it may be regarded as a systematic extension of the second-moment Finnis-Sinclair potential to include higher moments.

[1] R. Drautz and D.G. Pettifor, Phys. Rev. B 74, 174117 (2006).

MM 25.2　Wed 15:00　H6

Effects of local interactions on transport through interfaces — •FRANK FREIMUTH, DANIEL WORTMANN, and STEFAN BLÜGEL — Institut für Festkörperforschung, Forschungszentrum Jülich, Germany

The embedding technique provides a tool to calculate the Green function of the interface region of planar junctions suitable for application within DFT ab-initio studies of electronic transport. Our implementation of the embedding technique is based on the full-potential linearized augmented plane wave (FLAPW) method which does not make any approximations to the potential. In this talk, we give an outline of how the local Coulomb interaction may be taken into account within the embedding Green function approach through the local contribution to the self-energy. Wannier functions constructed from the DFT Bloch states of the interface provide a localized set of basis functions adequate for the calculation of many-body effects using many-body techniques formulated for lattice systems.

MM 25.3　Wed 15:15　H6

Conserving GW calculations for small metal clusters — •GEORGE PAL, YAROSLAV PAVLYUKH, HANS CHRISTIAN SCHNEIDER, and WOLFGANG HÜBNER — Fachbereich Physik, Technische Universität Kaiserslautern, P.O. Box 3049, 67663 Kaiserslautern, Germany

We present a GW-like approach for the quasiparticle energies and lifetimes of the closed-shell Na_4, Na_9^+ and Na_{21}^+ clusters. The screened Coulomb potential is constructed directly from the density-density correlation function, which is the functional derivative of a conserving single-particle Green's function with respect to an external potential. The density-density correlation function is obtained numerically by solving a quantum kinetic equation for the linear response of the system subject to a weak external perturbation. The conserving nature of our approach is shown by explicitly evaluating the f-sum rule. Analyzing the quasiparticle spectral functions, we find pronounced differences in the peak positions and broadenings when comparing our results with the self-consistent GW-RPA approach, which is not conserving at the two-particle level.

MM 25.4　Wed 15:30　H6

Is black phosphorous really a semiconductor? — •ALIM ORMECI and HELGE ROSNER — Max-Planck-Institut CPfS, Dresden

Black phosphorous in the A17 orthorhombic structure (space group 64) is known to be a narrow-band-gap semiconductor ($E_g = 0.3$ eV)

at ambient pressure. However, our recent electronic structure calculations based on various state-of-the-art first-principles, all-electron, full-potential codes have revealed that there is actually no gap in the electronic band structure of black phosphorous! Both LDA and GGA calculations give one small electron, and one small hole pocket around the **k**-point corresponding to $2\pi/b$ along the longest orthorhombic axis b. Thus, according to these very accurate calculations black phosphorous should be a compensated (semi)metal with very small $N(E_F)$ values in a wide range of unit cell volumes, at least between $0.90\,V_0$ and $1.15\,V_0$, where V_0 is the ambient pressure volume. The finding that the computed Fermi surface areas are very small has both computational and experimental implications. On the computational side, very fine sampling of the Brillouin zone is necessary in order to have a correct and converged result. On the experimental side, the implied low carrier concentration may introduce complications. We suggest new experiments such as photoemission, conductivity and de Haas-van Alphen measurements, to be performed on very pure, well-characterized single crystals of black phosphorous for testing the prediction regarding the existence of these small Fermi surfaces.

DFG Emmy Noether Programm is acknowledged for support.

MM 25.5　Wed 15:45　H6

The lattice structure of Zn, Cd, and Hg — NICOLA GASTON and •BEATE PAULUS — MPI fuer Physik komplexer Systeme, Noethnitzer Str. 38, 01187 Dresden, Germany

Mercury condenses at 233 K into the rhombohedral structure with a bond length a=3.005 Ang and an angle of 70.53 degree. In contrast, zinc and cadmium adopt the hexagonal close-packed (hcp) structure, but with an anomolous c/a ratio which is far from ideal hcp. Density functional methods fail to describe either of these structures accurately. An application of the method of increments [1] to these metals, including correlation via coupled cluster calculations on finite fragments of the solid, allows the systematic inclusion and comparison of the competing effects that leads to the observed structures [2].

[1] B. Paulus, Phys. Rep. 428, 1 (2006). [2] N. Gaston, B. Paulus, K. Rosciszewski, P. Schwerdtfeger and H. Stoll, Phys. Rev. B 74, 094102 (2006)

MM 25.6　Wed 16:00　H6

Boron/Carbon ordering in layered MB_2C_2 compounds — SERGII KHMELEVSKYI, PETER MOHN, and •JOSEF REDINGER — Inst. f. Allgemeine Physik, Vienna University of Technology, Getreidemarkt 9/134, A-1060 Vienna, Austria

Superconductivity in layered diboride dicarbide materials has been observed in YB_2C_2 and LuB_2C_2, but not in LaB_2C_2. Starting from our previous ab-initio DFT work on YB_2C_2 [1], where we showed that metallic conductivity in the stable $P4/mbm$ structure is due to Y d-bands partially hybridized with p_z-states from the boron-carbon planes, we present new results on the electronic structure of various layered boro-carbides such as CaB_2C_2, ScB_2C_2, SrB_2C_2, YB_2C_2, LaB_2C_2 and LuB_2C_2. We concentrate on the ordering of B and C in the layers and the impact of $d-p$ hybridization which seems to decide the actually observed structures. Except ScB_2C_2 which favours a 5-7 ring boron-carbon network ($Pbma$) all the others prefer 4-8 ring networks with alternating B and C atoms within the boron-carbon layer and a B-B (C-C) - like ($P4/mbm$) or B-C (C-B) - like ($I4/mcm$) layer stacking along the c-axis. Apparently, $d-p$ hybridization (YB_2C_2, LaB_2C_2 and LuB_2C_2) tips the scale in favour of $P4/mbm$, whereas CaB_2C_2 and SrB_2C_2 remain $I4/mcm$.

[1] S. Khmelevskyi, P. Mohn, J. Redinger, and H. Michor, Supercond. Sci. Technol. 18, 422-426, (2005).