

## MM 22 Electronic Properties II

Time: Wednesday 14:00–15:30

Room: IFW A

MM 22.1 Wed 14:00 IFW A

**Real-space methods in Density Functional Theory** — ●RALF MEYER — Theoretische Tieftemperaturphysik, Universität Duisburg-Essen, Campus Duisburg, D-47048 Duisburg, Germany

Density functional theory (DFT) has proven to be a reliable and accurate tool for the *ab-initio* calculation of materials properties. The most popular approach to the solution of the DFT equations is probably the plane-wave method. While a plane-wave basis is very efficient for dense periodic systems like crystalline solids, it is less suitable for the description of non-periodic systems like clusters. Moreover, the necessity to perform Fourier-transforms hampers the efficiency of the plane-wave method on massively parallel computers. These problems are avoided by real-space approaches like the finite-element or finite difference method that directly discretize the DFT equations in real space. In this presentation, calculations of metallic nanoclusters using a newly developed real-space code are shown and compared with corresponding results obtained with the plane-wave method.

MM 22.2 Wed 14:15 IFW A

**The fundamental gap in reduced-density-matrix-functional theory** — ●N. HELBIG<sup>1</sup>, N.N. LATHIOTAKIS<sup>1</sup>, M. ALBRECHT<sup>2</sup>, and E. K. U. GROSS<sup>1</sup> — <sup>1</sup>Freie Universität Berlin, Arnimallee 14, 14195 Berlin — <sup>2</sup>Theoretical Chemistry FB 08, University of Siegen, 57068 Siegen

We present a novel method for calculating the fundamental gap. To this end, reduced-density-matrix-functional theory is generalized to fractional particle number. For each fixed particle number,  $M$ , the total energy is minimized with respect to the natural orbitals and their occupation numbers. This leads to a function,  $E_{\text{tot}}^M$ , whose derivative with respect to the particle number has a discontinuity identical to the gap. In contrast to density functional theory, the energy minimum is generally not a stationary point of the total-energy functional. Numerical results are presented for alkali atoms, for small molecules and ionic periodic systems.

[1] N. Helbig, N.N. Lathiotakis, M. Albrecht, E.K.U. Gross, cond-mat/0504436

MM 22.3 Wed 14:30 IFW A

**Reduced-density-matrix-functional theory for the homogeneous electron gas** — ●N. N. LATHIOTAKIS, N. HELBIG, and E. K. U. GROSS — Freie Universität Berlin, Arnimallee 14, 14195 Berlin

Reduced-density-matrix-functional theory (RDMFT) is one possible way to treat electron correlation beyond density-functional theory. One of the drawbacks of the first generation RDMFT functionals is their failure to reproduce the correlation energy of the spin-unpolarized homogeneous electron gas (HEG). Recently, new RDMFT functionals were introduced which considerably improve the results for atoms and molecules. We apply these functionals to the HEG and show that they also improve dramatically the results obtained for the HEG: On one hand, they give correlation energies closer to the exact ones and, in contrast to the first-generation functionals, they properly yield a finite jump of the HEG momentum distribution.

Furthermore, we generalize the second-generation functionals in such a way that they reproduce the correlation energy of the HEG exactly over the whole range of electron densities. We discuss ways to apply the resulting functionals to both finite and inhomogeneous periodic systems.

MM 22.4 Wed 14:45 IFW A

**The intrinsic defect structure of  $\text{Al}_{1-x}\text{B}_2$  – an ab initio electronic structure study** — ●KATRIN KOCH, YURI GRIN, and HELGE ROSNER — MPI CPFS Dresden

Ab initio calculation of phase diagrams is still in its very early stages. For an outset towards new developments, we have chosen the simple hexagonal system  $\text{AlB}_2$ , which is nevertheless very interesting due to its close relation to the surprising superconductor  $\text{MgB}_2$ . Up to now, the synthesis of stoichiometric  $\text{AlB}_2$  has been impossible: grown in aluminium flux, a composition between  $\text{Al}_{0.9}\text{B}_2$  (from x-ray refinement) and  $\text{Al}_{0.85}\text{B}_2$  (from mass density measurements) has been found [1]. Here, we present band structure calculations within the local density approximation to investigate the structural stability in the phase equilibrium  $\text{AlB}_2 \rightleftharpoons \text{Al}_{1-x}\text{B}_2 + x \cdot \text{Al}$ . The defects are treated using the coherent poten-

tial approximation (CPA). Taking into account the full lattice relaxation depending on  $x$ , we find a stable energy minimum for the composition  $\text{Al}_{0.85}\text{B}_2$ . This is in excellent agreement with the experimental findings and explains the nonstoichiometric composition of present  $\text{AlB}_2$  samples. The influence of the defects on the electronic properties will be discussed. [1] U.Burkhardt *et al.* Journal of Solid State Chemistry **177**, 389, (2004)

MM 22.5 Wed 15:00 IFW A

**The highly distorted hcp lattices of Zinc and Cadmium: Comparison of different ab-initio approaches** — ●BEATE PAULUS<sup>1</sup>, KRZYSZTOF ROSCISZEWSKI<sup>2</sup>, PRIYA SONY<sup>3</sup>, ULRICH WEDIG<sup>4</sup>, and MARTIN JANSEN<sup>4</sup> — <sup>1</sup>MPI for the Physics of complex Systems, Dresden, Germany — <sup>2</sup>Institute of Physics, Jagellonian University, Krakow, Poland — <sup>3</sup>Institute of Technology, Mumbai, India — <sup>4</sup>MPI for Solid State Research, Stuttgart, Germany

Among the metallic elements crystallizing in a hexagonal closed packed structure, Zn and Cd are unusual because of the significant increase of the  $c/a$  ratio. Attempts to explain this distortion theoretically suffer from the fact that the calculated properties vary significantly with the method used. In order to investigate the peculiarities and the reliability of the different methods, ground-state properties like cohesive energy, the lattice constants and the elastic constants were calculated for Zn and Cd using the Hartree-Fock method, various density functionals and hybrid methods. In addition calculations were performed for Mg as a reference system with the ideal hcp structure. The dependence of the results on the computational methods and parameters gives further insight into the bonding mechanisms leading to the distortions in Zn and Cd and helps to judge the reliability of computed electron density maps to interpret experimental results.

MM 22.6 Wed 15:15 IFW A

**Lifshitz-transitions in Osmium under pressure** — ●DANIELA KOUDELA, KLAUS KOEPERNIK, ULRIKE NITZSCHE, and MANUEL RICHTER — IFW Dresden

The search for Lifshitz-transitions [1] is a recent subject of interest. Occelli *et al.* claimed, that they found evidence for a Lifshitz-transition in Osmium [2]. To explore this hypothesis from the theoretical side, we did very accurate first principle calculations applying the DFT-based bandstructure code FPLO [3]. From the resulting bandstructure, Fermi surfaces, and total energies we conclude, that Osmium undergoes three Lifshitz-transitions in the pressure range between 0 GPa and 150 GPa, which should be invisible in the elastic properties.

[1] I.M. Lifshitz, Zh. Eksp. Teor. Fiz. 38, 1569 [Sov. Phys. JETP 11, 1130 (1960)].

[2] F. Occelli, D.L. Farber, J. Badro, C.M. Aracne, D.M. Teter, M. Hanfland, B. Canny and B. Couzinet, Phys. Rev. Lett. 93, 095502 (2004).

[3] K. Koepernik and H. Eschrig, Phys. Rev. B 59, 1743 (1999); www.fplo.de.