# HL 43: Electronic Structure and Atomistic Modeling

Time: Wednesday 14:00–15:45 Location: H14

HL 43.1 Wed 14:00 H14

**Does the KLI approximation work for current-density-functional theory?** — •Marc Siegmund and Oleg Pankratov — Lehrstuhl für Theoretische Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7/B2, 91058 Erlangen, Germany

Orbital exchange-correlation functionals which depend explicitly on the Kohn-Sham orbitals but only implicitly on the density became popular in the last years. These functionals systematically improve the description of many-body effects within density-functional theory. Among those, the optimized effective potential (OEP) method is often employed which expresses the exchange-correlation potential as a solution of complicated integral equations. Due to the complexity of these equations, a simplification known as the Krieger-Li-Iafrate (KLI) approximation is widely used in practice.

Recently, the OEP integral equations and the KLI approximation have been derived for current-density-functional theory (CDFT) [1]. Using a one-dimensional model system, we discuss the applicability of the KLI approximation in this case. A numerical example shows, that the solution of the CDFT-KLI equations may produce the exchange-correlation vector potential which leads to violation of the continuity equation. On the contrary, the solution of the full CDFT-OEP equations does not suffer from this shortcoming.

[1] S. Pittalis, S. Kurth, N. Helbig, and E.K.U. Gross, Physical Review A **74**, 062511 (2006)

HL 43.2 Wed 14:15 H14

**Electronic properties of rolled-up materials** — •Carmine Ortix and Jeroen van den Brink — Leibniz-Institute for Solid State and Materials Research Dresden, D-01171 Dresden, Germany

The success achieved in modern nanotechnology has made it possible to develop systems having fairly complex geometrical shapes. Typical examples are the so-called rolled-up nanotubes which mimic the cylindrical geometry of a radial crystal. In this talk we will discuss the electronic properties of a rolled-up two-dimensional electron gas. The nature and energy dispersion of the quantum states reflect the interplay between the typical length scales of the problem. In addition we will show that the effect of an external magnetic field adds a new degree of freedom to manipulate the quantum states of the carriers.

HL 43.3 Wed 14:30 H14

**Exploring the unusual diffusion of N adatoms on GaAs(001) using first principles calculations** — •Hazem Abu-Farsakh and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, 40237 Düsseldorf, Germany

The large band-gap bowing resulting from the incorporation of N in GaAs has attracted a considerable interest recently for various applications including e.g. infrared laser diodes. However, epitaxial growth of dilute nitride alloys is hampered by several challenges. A key issue is the low solubility of N in this material system, which requires growth conditions far away from equilibrium. To optimize such conditions it is crucial to employ accurate simulation techniques. Key input quantities include diffusion paths and barriers on the growing surface. To determine these parameters we first employed *ab-initio* calculations to map the potential energy surface (PES) of N on GaAs(001) surface. Our results reveal that the energy landscape is highly complex and multivalued in nature. A detailed analysis showed that this is a consequence of the high reactivity of the N adatoms causing large surface relaxations. A consequence of this finding is that the conventional PES mapping approach dramatically fails. We therefore propose an alternative approach that allows us to identify the diffusion coefficients and the activation barriers over the entire relevant temperature range. Our results show a completely unexpected interplay of localization within the reconstructed surface unit cell that prevents equilibration and high mobility inside it guaranteeing the incorporation on the desired substitutional sites.

HL 43.4 Wed 14:45 H14

**Tight-binding theory of $Cd_xZn_{1-x}Se$ semiconductor alloy nanocrystals** — •Daniel Mourad and Gerd Czycholl — Institut für Theoretische Physik, Universität Bremen

For a wide class of semiconductor materials alloys of the type $A_xB_{1-x}$ can be realized, e.g. $Cd_xZn_{1-x}Se$, $Si_xGe_{1-x}$, $Al_xGa_{1-x}N$, $Ga_xIn_{1-x}N$, and many others. These substitutional alloys find widespread applications, in particular in nanoelectronic devices like quantum wells, quantum wires and quantum dots, as the band gap varies continuously with x, and therefore a band structure tayloring is possible by variation of the concentration. To calculate the electronic properties of such semiconductor alloys we start from multiband ($sp^3$) tight-binding (TB) models for the pure bulk semiconductor materials A and B and perform ensemble averaged finite supercell calculations. Alternatively, we apply the coherent potential approximation (CPA) to calculate and compare the configurationally averaged electronic density of states and effective band structure. These treatments allow for an intrinsic reproduction of band bowing effects as a function of the concentration x and lead to finite lifetime effects due to the loss of translational invariance, contrary to much simpler mean-field approaches like the virtual crystal approximation (VCA). As an up-to-date application, we have in particular investigated $Cd_xZn_{1-x}Se$ nanocrystals. We compare our results to experimental ones by combining these treatments with the recently developed TB models of nanostructures. Finally, we discuss the proper choice of material parameters for these systems.

HL 43.5 Wed 15:00 H14

**The Atomistic-Continuum Modeling of Short Pulse Laser Interaction with Semiconductors** — •Dmitriy Ivanov, Baerbel Rethfeld, and Vladimir Lipp — Physics Department, Technical University of Kaiserslautern, Kaiserslautern, Germany

The understanding of fundamental mechanisms behind the sub-wave length surface modification on semiconductors is of a great importance for Information Technologies. However, strong laser-induced phase perturbations, occurring under conditions of nonequilibrium between free laser-generated carriers and phonons, make the experimental and theoretical study of short pulse laser nanostructuring on semiconductors difficult. Previously, the atomistic-continuum approach for modeling of short-pulse laser interactions with metals have been proven as an efficient tool when studying processes of laser melting, ablation, and nanostructuring on metals.

In present work, a computational technique that combines the advantages of different approaches into the atomistic-continuum model for semiconductors is developing on the example of Si. In the combined model, 1) the kinetics of fast non equilibrium phase transformations is treated at atomic level with Molecular Dynamics method, and 2) the description of laser light absorption by free carriers, their transport dynamics, and strong laser-induced non equilibrium between free carriers and phonons are accounted for in the continuum part by means of free carrier dynamics model.

HL 43.6 Wed 15:15 H14

**Intrinsic *n*-type Behavior in Transparent Conducting Oxides: A Comparative Hybrid-Functional Study of $In_2O_3$, $SnO_2$, and ZnO** — •Péter Ágoston[1], Karsten Albe[1], Risto M. Nieminen[2], and Martti J. Puska[2] — [1]Technische Universität Darmstadt, Institut für Materialwissenschaft, Petersenstr. 32, 64287 Darmstadt — [2]Department of Applied Physics, Helsinki University of Technology, FIN-02015 TKK, Finland

We present a comparative study of point defects in $In_2O_3$, $SnO_2$ and ZnO based on the hybrid-functional method within the density functional theory (DFT). For $In_2O_3$ and $SnO_2$, our results provide strong evidence of shallow donor states at oxygen vacancies. The formation energies of oxygen vacancies are low both for the doubly positive and neutral charge states. In comparison with the semilocal exchange-correlation approximations in DFT the hybrid-functional method lowers strongly the formation energy of the positive charge state and keeps that of the neutral state nearly intact. The trend is analyzed in terms of changes in the lattice relaxation energy and the electron energy levels near the band gap. The existence of shallow donor states at oxygen vacancies and the consequent *n*-type conductivity are in line with experimental findings. The results invalidate some former theoretical interpretations.

HL 43.7 Wed 15:30 H14

**Semiconductors and oxides studied using relativistic exact-exchange implemented within the multiple scattering KKR formalism** — •Diemo Ködderitzsch and Hubert Ebert — Ludwig-Maximilians-Universität München, Department Chemie und

Biochemie, Physikalische Chemie, Butenandtstraße 11, D-81377 München, Germany

In the *systematic* development of new exchange-correlation (xc) functionals in density functional theory the so called orbital dependent xc-functionals have emerged and are now extensively studied. Here we give a formulation of relativistic exact-exchange (REXX) as an approximation to the xc-functional subsequently used in a multiple-scattering KKR Green's function implementation. Both core and valence states are treated on the same footing in an all electron approach. The REXX used for the valence states is reformulated in terms of the electronic Green's function. Numerical four-component wave functions for the description of the ingredients of the REEX integral equation are employed. We present and discuss the application of the formalism to semiconductors and oxides.