

HL 16: Theory: Metal-insulator transitions / Electronic structure calculations

Time: Monday 15:30–18:00

Location: H13

HL 16.1 Mon 15:30 H13

Robust Nodal Structure of Landau Level Wave Functions Revealed by Fourier Transform Scanning Tunneling Spectroscopy — K HASHIMOTO^{1,2}, T CHAMPEL³, S FLORENS⁴, C SOHRMANN⁵, J WIEBE⁶, Y HIRAYAMA^{1,2}, ●RA RÖMER⁵, R WIESENDANGER⁶, and M MORGENSTERN⁷ — ¹Tohoku University, Sendai, Japan — ²JST, ERATO Nuclear Spin Electronics Project, Sendai 980-8578, Japan — ³Université Joseph Fourier Grenoble I / CNRS UMR 5493, Grenoble, France — ⁴CNRS and Université Joseph Fourier, Grenoble, France — ⁵University of Warwick, Coventry, UK — ⁶Institute of Applied Physics, Hamburg University, Hamburg, Germany — ⁷RWTH Aachen University, Aachen, Germany

Scanning tunneling spectroscopy is used to study the real-space local density of states (LDOS) of a two-dimensional electron system in magnetic field, in particular within higher Landau levels (LL). By Fourier transforming the LDOS, we find a set of n radial minima at fixed momenta for the n th LL. The momenta of the minima depend only on the inverse magnetic length. By comparison with analytical theory and numerical simulations, we attribute the minima to the nodes of the quantum cyclotron orbits, which decouple in Fourier representation from the random guiding center motion due to the disorder. Adequate Fourier filtering reveals the nodal structure in real space in some areas of the sample with relatively smooth potential disorder.

HL 16.2 Mon 15:45 H13

A functional renormalization group approach for treating interactions in disordered electron systems — ●CHRISTIAN SEILER^{1,2} and FERDINAND EVERS^{1,2} — ¹Institut für Nanotechnologie, Karlsruher Institut für Technologie, Karlsruhe, Germany — ²Institut für Theorie der Kondensierten Materie, Karlsruher Institut für Technologie, Karlsruhe, Germany

We propose an approach to treat the effects of interactions in disordered electron systems on a numerical level. The idea is to solve the non-interacting disorder problem for a given disorder realization exactly. We then use the functional renormalization group method to introduce interactions on a perturbative level. In contrast to usual applications of the fRG, we formulate it in terms of the eigenfunctions of the disordered non-interacting Hamiltonian. Disorder averaging of physical quantities is performed as the final step. The main advantage of our approach is that we are able to treat disorder exactly from a numerical point of view. In fRG applications for clean systems the number of active degrees of freedom is reduced by projecting momenta near the Fermi surface to certain spots on this surface. Disordered systems do not lend themselves to such a treatment since momentum no longer is a good quantum number. Here, the challenge is to find another appropriate decimation technique. We devise, compare and discuss several candidates for such disorder-adapted decimation schemes.

HL 16.3 Mon 16:00 H13

Dependence Of Physical Properties Of Materials On The Approximations For The Exchange-Correlation Potential — ●ARCESIO CASTANEDA M., ALDO HUMBERTO ROMERO C., SANGEETA SHARMA, JOHN KAY DEWHURST, and EBERHARD GROSS — Max-Planck-Institut für Mikrostrukturphysik Weinberg 2, D-06120 Halle, Germany

Density Functional Theory (DFT) is in principle exact, but the quality of the results obtained using it, critically depend upon the approximation employed for the exchange-correlation functional. There exist a plethora of exchange-correlation functionals with increasing complexity and computational cost. However, increasing complexity does not necessarily imply better description of material properties. With this in mind, in the present work we analyze the structural, electronic and optical properties of 14 different semiconductors with 16 different exchange-correlation functionals (LDA and GGA type) using the libxc library and the all electron Elk code [1,2]. We discuss different trends and try to understand the effects of the studied functionals on the measured properties. We further propose regimes of application for the considered functionals depending on the property of interest.

[1] M.A.L. Marques, M.J.T. Oliveira and T. Burnus, Libxc: a library of exchange and correlation functionals for density functional theory, Comput. Phys. Commun. 183, 2272 (2012).

[2] K. Dewhurst, S. Sharma, L. Nordström et. al., The Elk FP-LAPW Code, <http://elk.sourceforge.net/>.

HL 16.4 Mon 16:15 H13

Dynamical processes and temperature effects in semiconductor nanoclusters — PENG HAN and ●GABRIEL BESTER — Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, 70569 Stuttgart, Germany.

Electron-phonon interactions in colloidal semiconductor quantum dots consisting of thousands of atoms are calculated using first principles density functional theory (DFT) and the frozen-phonon approach. In the computation, the electronic states and the change of the potentials caused by a phonon induced distortion of the lattice are self-consistently calculated using DFT; the electron-phonon interaction matrix elements are then obtained using perturbation theory. Using the electron-phonon coupling matrix elements obtained from this approach, we study the electronic relaxation processes in colloidal semiconductor nanoclusters (NCs) via the Liouville-von Neumann equation including a phenomenological Lindblad decay term. We observe a decaying Rabi oscillation with a period of tens of fs, corresponding to emission/absorption of a phonon, and with a decay rate that is dominated by the phonon lifetime. To estimate the phonon lifetime in NCs, we perform *ab initio* molecular dynamics simulations of a Si₁₀H₁₆ cluster and extract the time evolution of the energy of selected vibrational modes from the energy auto-correlation functions. We find vibrational cooling times of are around 1 ps for pure Si modes, which are close to the phonon lifetimes in bulk Si.

HL 16.5 Mon 16:30 H13

Ab initio simulation of crystallization in phase change materials — ●IDER RONNEBERGER¹, YAN LI¹, WEI ZHANG¹, SEBASTIANO CARAVATI², ESHET HAGAI², MICHELE PARRINELLO², and RICCARDO MAZZARELLO¹ — ¹Institut für Theoretische Physik, RWTH Aachen — ²Comp. Science, Dep. of Chem. and Appl. Biosciences, ETH Zürich

The microscopic understanding of the crystallization processes in the technologically relevant phase change materials (PCM) is desirable, in that it could eventually lead to improved properties for applications. Ab initio Molecular Dynamics (AIMD) simulations are very useful to investigate these processes and plenty of atomistic studies were conducted in the field of PCM research. However typical simulation times of AIMD are of the order of 1 ns or less, so that observation of long-time processes and rare events (such as crystallization at low temperature) is computationally not affordable. A new efficient sampling method, called metadynamics, was introduced a decade ago, which can accelerate the dynamics by biasing with history-dependent potentials and lead to an estimation of the free energy change during the process. In this study we employed the so called Well-Tempered version of metadynamics in combination with AIMD to study the crystallization of GeTe as a model representative of PCMs. Using a few selected reaction coordinates, models with up to 512 atoms were considered and the free energy change upon crystallization computed at 600 K. The results show that this method is a promising tool to determine nucleation barriers in PCMs. We plan to extend this study to different temperature ranges and other PCMs.

Coffee break

HL 16.6 Mon 17:00 H13

Metal-Insulator Transitions of Crystalline Phase-Change Materials — ●WEI ZHANG¹, ALEXANDER THIESS², PETER ZALDEN¹, RUDOLF ZELLER², PETER DEDERICHS², JEAN-YVES RATY³, MATTHIAS WUTTIG^{1,4}, STEFAN BLUEGEL^{2,4}, and RICCARDO MAZZARELLO^{1,4} — ¹RWTH Aachen, Germany — ²Forschungszentrum Jülich, Germany — ³University of Liege, Belgium — ⁴JARA, Germany

The study of metal-insulator transitions (MITs) in crystalline solids is a subject of paramount importance. Recently, a metal-insulator transition solely due to disorder has been observed experimentally in the crystalline phase-change material (PCMs) Ge₁Sb₂Te₄ (GST): upon annealing at temperatures T below 548K, the system shows insulating behavior due to Anderson localization; when annealing at higher T , it exhibits metallic properties. In this work, we present an ab initio

Density Functional Theory study of this effect. By considering a set of very large models of GST containing one to several thousand atoms and different degree of disorder, we identify the microscopic mechanism which localizes the electron wavefunctions near the Fermi energy in the insulating phase as due to vacancy clustering. The ordering of these vacancy clusters upon annealing eventually drives the system to the metallic phase. Our results about crystalline PCMs could help to extend the capacity of current data storage devices based on PCMs, which only utilize the electrical contrast between the crystalline and the amorphous phase.

HL 16.7 Mon 17:15 H13

Large-Scale Electronic Structure calculations of Semiconductor Nanostructures using Atomic Effective Pseudopotentials

— •FRANK ZIRKELBACH, JAIRO RICARDO CARDENAS, PIERRE-YVES PRODHOMME, PENG HAN, ROBY CHERIAN, and GABRIEL BESTER — Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, D-70569 Stuttgart, Germany

In the presented scheme [1], the Schrödinger equation of an electronic system is solved within an effective single-particle approach utilizing atomic effective pseudopotentials [2], which are derived from screened local effective crystal potentials obtained from self-consistent density functional theory calculations on elongated and slightly deformed bulk structures. The use of these potentials allows to bypass a self-consistent procedure, which drastically reduces the computational effort. Furthermore, iterative solvers can be used to focus only on a few eigenstates of interest, e.g., states in the vicinity of the band gap of a semiconductor. Hence, this approach enables first-principles investigations of the electronic structure of semiconductor nanostructures consisting of ten thousands of atoms. In addition to the non-local contribution of the *ab initio* pseudopotential to reconstruct the full crystal potential, a real space treatment scaling linearly with the number of atoms is used to include spin-orbit effects.

[1] G. Bester et. al., unpublished (2012).

[2] J. R. Cárdenas and G. Bester, Phys. Rev. B **86** (2012).

HL 16.8 Mon 17:30 H13

Calculation of branch points and band offsets for cubic $\text{Ga}_x\text{Al}_{1-x}\text{N}$ — •DANIEL MOURAD — Institut für Theoretische Physik, Universität Bremen

The anisotropic valence band offset (VBO) across the interface between two materials is an important material parameter and can ap-

proximately be calculated from the branch points (BPs, aka charge neutrality levels) of the constituent materials. $\text{Ga}_x\text{Al}_{1-x}\text{N}$ is a technologically important semiconductor alloy and often used as barrier material in optoelectronic devices. Nevertheless, most work and available data concentrates on the hexagonal modification, while there is considerably less data for the zincblende phase of the alloy. The latter also shows an interesting direct to indirect band gap transition on the Al-rich side, which makes it an interesting model system for the calculation of concentration-dependent properties.

We show how the concentration-dependent BP of the disordered $\text{Ga}_x\text{Al}_{1-x}\text{N}$ alloy can be calculated within a combination of a suitable tight-binding model and the coherent potential approximation (CPA). We then analyse the resulting VBOs for several material combinations and interface orientations and discuss the extension to the wurtzite phase and further nitride alloys like $\text{In}_x\text{Ga}_{1-x}\text{N}$.

HL 16.9 Mon 17:45 H13

Density Functional Theory Investigation of inner-Surface Methylated Aluminosilicate Nanotubes — •JOSHUA ELLIOTT — University of Liverpool, Liverpool United Kingdom

We present a linear-scaling Density Functional Theory (LS-DFT) investigation into the electronic structure and stability of organic/inorganic hybrid Methyl-Aluminosilicate nanotubes (me-ALSi) as prepared and characterized in [1]. Due to the size of the considered systems (with unit-cells in excess of 350 atoms), we make use of the LS-DFT code ONETEP [2]. Following investigation of the convergence of the results with respect to the ONETEP simulation setup (kinetic energy cutoff, number and radius of the in situ optimised basis-set [2]), the effect of inner methyl incorporation on the structure of aluminosilicate nanotubes has been studied. We find that the lowest-energy tube structure has 13 unit repeat units in its circumference and a periodicity along tube axis in good agreement with available experimental data (8.0 Å[1]). We find that the presence of methyl groups does not inhibit the real space localisation of the Conduction Band (CB) and Valence Band (VB) on different sides of the nanotube cavity, nor the accumulation of positive (negative) charge at the outer (inner) surface of the tube, typical of Aluminosilicate (ALSi) nanotubes [3]. The methyl-induced shift on the me-ALSi VB and CB edges is finally quantified and suggested as an effective strategy towards doping of aluminosilicate interfaces.

[1] Phys. Chem. Chem. Phys., 13, 2, 744, (2010). [2] J. Chem. Phys. 122, 084119 (2005). [3] J. Phys.: Cond. Mat., 21, 195301 (2009).