HL 2: Electronic Structure Theory

Time: Monday 10:15–11:45 Location: POT 51

HL 2.1 Mon 10:15 POT 51

Quasiparticle band offsets at heterojunctions from GW superlattice calculations — •Christoph Freysoldt, Chandrima Mitra, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung, Düsseldorf

The alignment of electronic bands at heterointerfaces is a key parameter for the performance of a variety of electronic devices. Theoretical calculations are an important aid in disentangling the underlying mechanisms and in designing better interfaces. Yet, the predictive capability of modern electronic structure theory's workhorse, namely density functional theory (DFT), is limited due to the band gap problem in standard functionals. Many-body perturbation theory in the GW approximation offers a systematic way to improve upon DFT, but for practical purposes, many additional approximations must be employed that affect the absolute alignment of the GW self-energy. This severely restricts the possibility to obtain quasiparticle corrections for the heterointerface band offset from separate bulk calculations. We propose an alternative route which circumvents the transferability issues of absolute GW corrections. For this, relative GW corrections are determined for a superlattice. By choosing electronic marker levels in the valence band that are spatially well localized within either AlN or GaN, and by then correcting for the intraband dispersion of self-energy effects, we extrapolate the GW corrections of the band edges. Our results for zincblende AlN/GaN and AlP/AlAs show that using absolute GW corrections from separate bulk calculations gives errors of up to 40 % compared to the full GW calculation.

HL 2.2 Mon 10:30 POT 51

Many Body calculations of Band offsets in III-V semiconductors heterostructures — •Pierre-Yves Prodhomme and Gabriel Bester — Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1, 70569 Stuttgart, Germany.

Band offset are widely used to predict quantum properties of solid states. However most of the time these quantities are not calculated directly but rather rely on model for taking into account the effect of structure deformation on the band structure and a transitivity relation is assumed. Here we calculate directly the band offset of III-V heterostructures within the Many Body Perturbation Theory (in particular the GW approximation) for different strained unit cells in the stack. We propose different conditions under which the DFT computation and the deformation potential model are sufficient to obtain accurate band offsets in the case of III-V semiconductors. The validity of the transitivity relation according to the type of deformation and the type of semiconductor is discussed.

HL 2.3 Mon 10:45 POT 51

Vibrational properties of colloidal quantum dots — •Peng Han and Gabriel Bester — Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, 70569 Stuttgart, Germany.

To investigate the effects of carrier relaxation and dephasing via electron phonon coupling, the vibrational properties of the III-V semiconductor quantum dots are studied by density-functional perturbation theory (DFPT). Based on our calculation, decreasing the quantum dots diameters from 3.4 to 2.6 nm results in a blue shift of the longitudinal acoustic and optical vibration modes. The surface vibration modes are found to appear in the gap between the acoustic and the optical branches. In addition, the vibrational properties of the InAs/InP core/shell quantum dots are studied by projecting the vibrational eigenmodes onto the core and the shell atoms separately. The longitudinal acoustic modes of the core and shell atoms are found to be merged together, while the other modes remain distinct.

HL 2.4 Mon 11:00 POT 51

Optimized basis sets for coarse-grained electronic structure calculations of point defects — •Björn Lange, Christoph Freysoldt, and Jörg Neugebauer — Max-Planck Institut für Eisenforschung GmbH, 40237 Düsseldorf, Deutschland

Density-functional theory is a powerful tool to study the properties of point defects in the supercell approach. Yet, the size limitations make a description of the extended tails of defect states, especially for shallow defects, cumbersome. Atomic orbital basis sets are the method of choice to coarse-grain electronic structure calculations, but are in general not flexible enough for describing the unusual bonding situations, which occur in point defects. We employ a newly developed method that, based on a variational principle, allows to generate small atomic basis sets which optimally mimic the Kohn-Sham wavefunctions with a plane-wave basis set. We show that these basis sets accurately reproduce the underlying plane-wave calculation. We analyze how the atomic orbitals close to the defect are modified in comparison to their bulk counterparts. We are able to extend basis sets generated from small supercells and to reproduce the bandstructure of larger cells. Using this approach we construct and solve a reliable sparse model Hamiltonian for a shallow defect test system containing $10^3..10^4$ atoms.

HL 2.5 Mon 11:15 POT 51

EPR parameters of the dangling bond defect in crystalline and amorphous silicon: A DFT-study — •Gernot Pfanner, Christoph Freysoldt, and Jörg Neugebauer — Max-Planck Institut für Eisenforschung, Max-Planck-Strasse 1, D-40237 Duesseldorf

Thin-film a-Si:H solar cells are considered as low-cost alternatives to bulk crystalline silicon (c-Si) solar cells. A disadvantage of these devices is that their efficiency is severely limited by light-induced defects (Staebler-Wronski effect). In this context, electron-paramagnetic resonance (EPR) is a key technique to probe for the local atomic structure of defects with unpaired spins such as the silicon dangling bond. However, the assignment of the EPR signal to a specific defect structure requires comparison to theoretical models.

Using density-functional theory, we address structure-property relationships by combining systematic studies for idealized dangling-bond models in c-Si with a statistical analysis of a variety of dangling bonds in a-Si:H supercells. Our studies reveal the influence of the local geometry on sp-hybridization and delocalization. Yet, the structural variability of a-Si:H cannot be captured by these idealized defect models alone. Rather, our calculations indicate that a relatively broad distribution of dangling-bond like structures gives rise to the experimental signal supporting a recent re-evaluation of EPR parameters from multifrequency EPR.

HL 2.6 Mon 11:30 POT 51

Holographic view on nanostructure wave functions — •Gabriel Bester[1], Jie Peng[1], Wen Lei[2], Christian Notthoff[2], Axel Lorke[2], Dirk Reuter[3], and Andreas Wieck[3] — [1]Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, 70569 Stuttgart, Germany — [2]Department of Physics and CeNIDE, University of Duisburg-Essen, Lotharstraße 1, 47048 Duisburg, Germany — [3]Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum, Universitätsstraße 150, 44780 Bochum, Germany

In this contribution we demonstrate the possibility to influence the shape of the wave-functions in semiconductor quantum dots by the application of an external magnetic field B_z. The states of the so-called p-shell, which show distinct orientations along the crystal axes for $B_z = 0$ can be modified to become more and more circularly symmetric with increasing field. Their changing probability density can be monitored using magneto-tunneling wave function mapping. Calculations of the magneto-tunneling signals are in good agreement with the experimental data and explain the different tunneling maps of the p^+ and p^--states as a consequence of the different sign of their respective phases.

W. Lei *et al.*, Phys. Rev. Lett. **105**, 176804 (2010).