

HL 98: Electronic Structure Theory

Time: Friday 9:30–12:30

Location: EW 202

HL 98.1 Fri 9:30 EW 202

Defect levels hidden by the Kohn-Sham band gap — ●BOCKSTEDTE MICHEL — Theoretische Festkörperphysik, FAU Erlangen-Nürnberg, Staudtstr 7B2, 91058 Erlangen

Defects in semiconductors are decisive for the electronic properties. Furthermore they can implement Q-bits for quantum computing. To access the underlying physics, the accurate theoretical description of defect levels and excited states is highly desirable. Yet, the theoretical work horse, density functional theory (DFT) with (semi-)local XC-functionals, suffers from the well-known Kohn-Sham band-gap error. This not only affects defect states within the gap, but may turn otherwise localized ones into resonances outside the gap. Many-body perturbation theory (MBPT) on top of the DFT electronic structure was shown recently to yield excellent results for ionization levels and excited states, however, the latter problem of the DFT may easily hamper such calculations. Here we investigate this problem for a defect in SiC for the polytypes 3C and 4H with different band gaps using MBPT on top of DFT with LDA and HSE06 functionals. While in 4H-SiC G_0W_0 ionization levels for both functionals agree well, the proper defect states in 3C remain resonances within the LDA. Here simple ad-hoc corrections yield already good results.

HL 98.2 Fri 9:45 EW 202

Hybrid functionals in WIEN2k: implementation and applications — ●FABIEN TRAN¹, DAVID KOLLER¹, FERENC KARSAI¹, PETER BLAHA¹, and ANTIA S. BOTANA² — ¹Institute of Materials Chemistry, Vienna University of Technology, A-1060 Vienna Austria — ²Departamento de Física Aplicada, Universidade de Santiago de Compostela, E-15782 Santiago de Compostela, Spain

The screened and unscreened hybrid functionals were recently implemented into the WIEN2k code [1]. Results obtained with the hybrid functionals PBE0 and YS-PBE0 for the calculation of the F center in LiF and the electronic and magnetic properties of CrN will be presented. There will be also a discussion of the various approximations which can be done to make calculations with hybrid functionals faster, e.g., considering only the diagonal elements of the 2nd Hamiltonian [2] or using a reduced k-mesh for the screened Hartree-Fock potential.

[1] F. Tran and P. Blaha, Phys. Rev. B **83**, 235118 (2011).

[2] F. Tran, arXiv:1106.0434.

HL 98.3 Fri 10:00 EW 202

Implementation of NMR into the LAPW method — ●ROBERT LASKOWSKI and PETER BLAHA — Vienna University of Technology, Institute of Materials Chemistry, Getreidemarkt 9/165-TC, A-1060 Vienna, Austria

We present an full potential, all electron augmented plane wave (APW) implementation of the first-principle calculation of the NMR chemical shifts. In order to obtain the induced current we follow the perturbation approach [C. J. Pickard and F. Mauri, Phys. Rev. B **63**, 245101 (2001)]. The calculated all electron current is represented in traditional APW manner, namely we use Fourier representation in the interstitial region and spherical harmonics representation inside non-overlapping atomic spheres. The current is integrated using a pseudo charge technique of Weinert. The implementation is validated by comparison of the computed chemical shifts for sets of solids and molecules with available published data.

HL 98.4 Fri 10:15 EW 202

From long- to short-range correlations in the many-body perturbation theory — ●ANDRIS GULANS¹, TORBJÖRN BJÖRKMAN¹, NATALIA BERSENEVA¹, ARKADY KRASHENINNIKOV^{1,2}, and RISTO NIEMINEN¹ — ¹Aalto University School of Science, Espoo, Finland — ²University of Helsinki, Finland

Exfoliated layered solids commonly exhibit unusual properties in comparison to their bulk counterparts. Reliable theoretical studies of these materials often require more than just the standard density functional theory. Then, it is desirable to apply methods of the many-body perturbation theory, but they converge slowly with respect to the basis size. We argue that this problem stems from the electron-electron interaction cusp of correlated wavefunctions. Our analysis of the uniform electron gas shows that RPA correlation energies as well as GW quasiparticle energies converge as the negative third power of the cut-off

wavevector, and also a further asymptotic expansion is possible. This result is applied for a study of binding in 30 layered solids and the quasiparticle band structure of BN and MoS₂. Obtained exfoliation energies are surprisingly similar with the typical value of 20 meV/Å². The quasiparticle calculations show that the band gaps strongly depend on the width of the vacuum gap between periodic images of single layers, which is another long-range correlation effect along with the van der Waals interaction. The accuracy of these results is strongly influenced by the treatment of the short-range electron correlations.

HL 98.5 Fri 10:30 EW 202

Electronic and optical properties of cadmium fluoride: the role of many-body effects — ●GIANCARLO CAPPELLINI¹, JUERGEN FURTHMUELLER², FRIEDHELM BECHSTEDT², and EMILIANO CADELANO¹ — ¹SLACS-IOM-CNR and UniCA, Cagliari, Italy — ²IFTO-FSU, Jena, Germany

The electronic excitations and optical spectra of CdF₂ are calculated employing state-of-the-art techniques based on density functional theory and many-body perturbation theory. We use the perturbative GW scheme proposed by Hedin for the electronic self-energy to calculate single-particle excitation properties as the energy bands and the density of states (DOS). The electronic DOS near the gap region and the energy-band structure are compared with existing data from literature. The role of many-body effects turns out to be of fundamental importance for these single-particle properties. We show moreover that also for optical properties many-body effects, treated within the Bethe-Salpeter equation framework, are crucial to allow reasonable comparison with existing experimental spectra. We discuss the existence of a bound exciton located about 1 eV below the quasiparticle gap. For both, single-particle and two-particle effects, we explore the possibility of using simplified schemes and/or approximations which could reduce the computational effort, maintaining the physical results reliable. In addition, we also present preliminary results for the fluoride BaF₂ for comparison.

Coffee Break (15 min)

HL 98.6 Fri 11:00 EW 202

Derivation of effective atomic potentials as new type of pseudopotentials — ●JAIRO RICARDO CARDENAS, ROBY CHERIAN, and GABRIEL BESTER — Max Planck Institute for Solid State Research

We derive a new type of pseudopotentials from conventional norm-conserving pseudopotentials for the treatment of a large number of atoms. The pseudopotentials are not aimed at the calculation of the total energy, but of band edge states relevant for optical processes. We describe the pseudopotential construction and benchmark its quality and transferability by comparison to standard DFT calculations.

HL 98.7 Fri 11:15 EW 202

A comparison of density functionals for the charge transfer level of the N defect in ZnO — ●SUNG SAKONG, PETER KRATZER, and JOHANN GUTJAHR — Fakultät für Physik and Center for Nanointegration (CeNIDE), Universität Duisburg-Essen, Duisburg, Germany

Electronic structure of impurity states in semiconducting materials is a very popular research field in both science and industry. However, the most frequently employed density functional theory (DFT) method has a significant problem to reproduce the experimentally measured band gap. As a consequence, recently hybrid functionals are introduced to remedy the underestimated band gap.

We present a comparison of defect calculations between generalized-gradient-approximation (GGA-PBE) and hybrid functionals (HSE and PBE0) for the experimentally well characterized N impurity in ZnO [AIP Advances **1**, 022105 (2011)]. In addition, we test also empirical correction schemes with $+U$ and non-local potential [PRB **77**, 241201 (2008)] methods on top of the GGA functional. By referring all energy levels to the vacuum level of the corresponding method, we are able to compare the results. From the calculations, we notice that the charge transfer level (0/-) of N defects on the O site goes deeper into the gap in the methods that give a larger band gap, in good accordance with experiment and previous calculations [Appl. Phys. Lett. **95**, 252105 (2009)]. Moreover, we find the absolute positions of the charge transfer levels with respect to the vacuum levels to be less dependent

on the functionals than the band edges, because the charge states are determined from the more robust DFT total energies.

HL 98.8 Fri 11:30 EW 202

First-principles simulations of catalytic effects of the gold nanoparticle on the GaAs nanowire growth — ●YAOJUN DU, PETER KRATZER, SUNG SAKONG, and VOLKER PANKOKE — Fakultät für Physik and Center for Nanointegration

The interface between an Au nanoparticle and a GaAs nanowire can facilitate the nanowire growth due to a segregation of materials to the interface. Previous experimental studies have suggested that an Au nanoparticle alloyed with Ga atoms can supply Ga atoms to the interfacial growth zone. On the other hand, an Au nanoparticle can also absorb As_2 from the vapor phase during molecular beam epitaxy. This allows for a continuous supply of gallium and arsenic which is necessary for a GaAs nanowire growth. Employing density functional theory approaches, we have shown that an Au particle that can alloy with Ga atoms to form a stable surface is capable of catalytically dissociating As_2 impinging from the vapor phase. Moreover, relatively stable As-Ga species can form on the AuGa surface which could build up an As-Ga supply for growth at the interface. We are investigating the As diffusion within GaAs bulk crystal structures and along the interface between an Au nanoparticle and a GaAs nanowire. This should allow us to gain full insight on catalytic effects of the gold nanoparticle on the GaAs nanowire growth.

HL 98.9 Fri 11:45 EW 202

Tight binding in cylindrical coordinates for the electronic states of Si/Ge rolled-up nanotubes — ●GIOVANNI PIZZI¹, MICHELE VIRGILIO^{2,3}, GIUSEPPE GROSSO^{2,3}, SUWIT KIRAVITTAYA⁴, and OLIVER G. SCHMIDT⁴ — ¹Theory and Simulation of Materials, École Polytechnique Fédérale de Lausanne, Switzerland — ²NEST, Istituto Nanoscienze-CNR, Italy — ³Dipartimento di Fisica, Università di Pisa, Italy — ⁴Institute for Integrative Nanosciences, IFW Dresden, Germany

We have extended the $sp^3d^5s^*$ tight-binding model to the case of cylindrical symmetry in order to study the electronic states of multiwall rolled-up nanotubes, under the assumption of discrete rotational symmetry around the tube axis. We discuss the modifications that have to be applied to the standard tight-binding model so as to take into account the effects of the curvature on the hopping energies and on the spin-orbit coupling.

The input equilibrium positions of the atoms are obtained by means of continuum elasticity theory [1], and the electronic bands and states can be obtained with the code that we have developed for zincblende-like structures, using the parameters of Ref. [2]. The electronic band structure, the degeneracy liftings and the valley splitting in the conduction band of rolled-up Si/Ge nanotubes are discussed as an application.

[1] M. Grundmann, Appl. Phys. Lett. **83**, 2444 (2003).

[2] Y. M. Niquet, D. Rideau, C. Tavernier, H. Jaouen, and X. Blase,

Phys. Rev. B **79**, 245201 (2009).

HL 98.10 Fri 12:00 EW 202

Confinement effects on the vibrational properties of colloidal quantum dots — ●PENG HAN and GABRIEL BESTER — Max-Planck-Institut fuer Festkoerperforschung, Heisenbergstrasse 1, 70569 Stuttgart, Germany

Vibrational properties of colloidal III-V and II-VI quantum dots with thousand atoms are studied using first-principle density-functional theory (DFT) calculation. We describe the connection between the vibrational properties (including surface acoustic/optical modes, coherent acoustic modes, blue shifts for small radii and red shifts for large radii) and the structural changes induced by the surface. We can clearly ascribe most of these observations to the large relaxation of the clusters dominated by an inward relaxation of the surface penetrating deep inside the cluster of III-Vs and large distribution of bond length at the surface of II-VIs. These strong confinement effects tend to disappear for clusters with more than thousand atoms, where a small red shift of the Raman peak remains, due to a softening in response to undercoordination. The coherent acoustic modes, which have been viewed as the main cause for the bright-dark transition in the fine-structure splitting of quantum dots, are identified by our DFT calculation and found to agree well with the results from the Lamb model and experiment.

HL 98.11 Fri 12:15 EW 202

Extracting an effective band structure from supercell calculations on alloys and impurities: Evolution of the impurity band with clustering in GaN:P — ●VOICU POPESCU^{1,2} and ALEX ZUNGER³ — ¹Faculty of Physics, University Duisburg-Essen, 47048 Duisburg, Germany — ²Colorado School of Mines, Golden, Colorado 80401, USA — ³University of Colorado, Boulder, Colorado 80302, USA

While the supercell approach to defects and alloys enables to circumvent the limitations of those methods that insist on using artificially high symmetry, this step usually comes at the cost of abandoning the language of E versus \vec{k} band dispersion. We describe a computational method that maps the energy eigenvalues obtained from large supercell calculations into an effective band structure (EBS) and recovers an approximate $E(\vec{k})$ for alloys. Making use of supercells allows one to model a random alloy $\text{A}_{1-x}\text{B}_x\text{C}$ by occupying the sites A and B via a coin-toss procedure affording many different local environments to occur (polymorphic description). We present the supercell EBS methodology and apply it to study the evolution of the impurity band appearing in the dilute GaN:P alloy. We treat both the perfectly random case as well as the non-random microstructures formation, and investigate how their appearance is reflected in the EBS. It turns out that the EBS is extremely sensitive in determining the critical disorder level for which delocalised states start to appear in the intermediate band. In addition, the EBS allows us to identify the role played by atomic relaxation in the positioning of the impurity levels.