

O 67: Theory: General

Time: Wednesday 18:15–20:30

Location: Poster A

O 67.1 Wed 18:15 Poster A

Excited-state lifetimes in binuclear copper centers calculated from first principles — •MARTIN ROHRMÜLLER¹, MARIA NAUMOVA^{1,2}, MICHAEL RÜBHAUSEN², GERALD HENKEL¹, and WOLF GERO SCHMIDT¹ — ¹Universität Paderborn, 33098 Paderborn, Germany — ²Universität Hamburg, 20355 Hamburg, Germany

Proteins containing copper sulfur complexes play a key role for electron transfer in biological systems. In order to explore the interplay between the structural and electronic degrees of freedom in these systems, smaller biomimetic model complexes such as $[\text{Cu}_2((\text{NGuaS})_2)_2]^{2+}$ [1] are investigated.

In this presentation we explore the electronic structure and in particular the lifetime of electronic excitations in $[\text{Cu}_2((\text{NGuaS})_2)_2]^{2+}$. To that end the imaginary parts of the electron self-energies – related to the quasi-particle lifetime due to electron-electron interaction – are calculated within many-body perturbation theory based on the density functional theory electronic structure [2].

We analyze the metal to ligand charge transfer (MLCT) excitations of the model complex including structural relaxations and discuss in detail the numerical stability and convergence of the calculated electronic self-energy with respect to the simulation parameters.

[1] A. Neuba *et al.* *Angew. Chem. Int. Ed.*, **51**, 1714 (2012).

[2] A. Marini *et al.* *Phys Rev. B* **66**, 161104R (2002).

O 67.2 Wed 18:15 Poster A

Interplay of structural and electronic properties in thin-film absorbers — •THOMAS BISCHOFF¹, CLAUDIA SCHNOHR², and SILVANA BOTTI¹ — ¹Institut für Festkörperteorie und theoretische Optik, 07743 Jena, Germany — ²Institut für Festkörperphysik, 07743 Jena, Germany

During the past years, $\text{Cu}(\text{In,Ga})(\text{Se,S})_2$ (CIGS) thin-film solar cells have emerged as a technology that could challenge the current hegemony of silicon solar panels. CIGS compounds conserve to a very high degree their electronic properties in a large non-stoichiometric range and are remarkably insensitive to radiation damage or impurities. The family of kesterites $\text{Cu}_2\text{ZnSe}(\text{S,Se})_4$ (CZTS) exhibits very similar electronic properties. Moreover, kesterites have the clear advantage of being composed of abundant, non-toxic, less expensive chemical elements. However, the efficiency of CZTS solar cells is about 50% smaller than the one of CIGS solar cells.

The origin of the exceptional electronic properties and the defect physics of these compounds and their alloys is still far from being completely understood, despite the large amount of experimental and theoretical work dedicated to that purpose.

We present here self-consistent GW calculations of the dependence of the band gap on internal distortions. Combined with EXAFS measurements, our calculations allow to quantify the structural contributions to the band gap bowing of alloys of these families.

O 67.3 Wed 18:15 Poster A

Efficient Moller-Plesset perturbation theory for extended systems — •THEODOROS TSATSOULIS and ANDREAS GRÜNEIS — Max-Planck-Institute for Solid State Research, Stuttgart

Kohn-Sham density functional theory is one of the most popular methods used in material science. However, many functionals cannot accurately determine the energetics of solids and surfaces. Furthermore, there is no systematic way to improve upon the functionals. The wave-

function based treatment of electronic correlation constitutes a hierarchy of methods that allows one to systematically approximate the many-body nature of the true ground state wave-function, however, with a large computational cost. The latter stems to a large extent from the unfavorable scaling of the computational cost with the number of virtual states. It is therefore critical to span only the relevant parts of the virtual space for the implementation of efficient wave-function based methods. We consider an approach whereby the occupied orbitals are converged in a plane wave basis, whereas the virtual space is then constructed using pseudized Gaussian orbitals expanded in plane waves. This approach allows for an efficient implementation of wave-function based methods. Results are shown for water adsorption on surfaces at the level of Møller-Plesset perturbation theory within the projector-augmented-wave method as implemented in VASP [1].

[1] Marsman *et al.*, *The Journal of Chemical Physics*, **130**, 184103 (2009)

O 67.4 Wed 18:15 Poster A

Implementation of electron-phonon coupling in the KKR formalism — •CARSTEN EBERHARD MAHR, MICHAEL CZERNER, CHRISTIAN FRANZ, and CHRISTIAN HEILIGER — Justus-Liebig-University, Giessen, Germany

Electron-phonon coupling is one of the main incoherent inelastic scattering mechanisms in a wide variety of crystalline material systems at room temperature. Therefore, it is necessary to incorporate those effects in any realistic calculation of thermoelectric properties. We do so by extending our density functional theory (DFT) based Korringa-Kohn-Rostocker (KKR) Green's function formalism code.

By approximating the Fröhlich-type interaction with a self-energy $\Sigma_{\text{eph}} = -i\frac{\hbar}{2\tau}$ we can compute the dressed propagator G by solving Dyson's equation $G = G_{\text{ref}} + G_{\text{ref}} \cdot (\Delta V + \Sigma_{\text{eph}}) \cdot G$, where G_{ref} is an arbitrary (though typically repulsive) reference system. The electron-phonon scattering time τ may be extracted from e.g. electron linewidth calculations.

We present mathematical and implementational details of the beforementioned calculational scheme for non-equilibrium properties in the KKR basis set and discuss its physical validity by evaluating resistivity characteristics of simple transport systems.

O 67.5 Wed 18:15 Poster A

Deblurring of Photoelectron Diffraction (XPD) Signals — •CHRISTOPHER KOHLMANN, TOBIAS LÜHR, CHRISTOPH KEUTNER, DOMINIQUE KRULL, and CARSTEN WESTPHAL — Experimentelle Physik I, TU Dortmund, Germany, Otto-Hahn-Str. 4, 44221 Dortmund

The photoelectron diffraction (XPD) is a established and appropriate method for the analysis of the structure of surface and interfaces. In order to regain the structural information out of the experimental data, simulations have to be performed. Precise reconstruction of the atomic structure can be determined by comparing the experimental and simulated data. We use a self made automated genetic algorithm to gain a better performance in quantity and quality. In order to reduce the influence of experimental artefacts, we are going to perform deblurring procedures on the experimental patterns. Therefore, the kernel function and the real diffraction effects of the sample need to be deconvoluted. Hence, the kernel function as well as a suitable data sampling method have to be found. This deconvolution method can also be applied on other experimental methods, like STM and PEEM.