

O 20: Poster Monday: Electronic Structure

Time: Monday 17:45–20:00

Location: Poster F

O 20.1 Mon 17:45 Poster F

CuI as Potential *p*-type Transparent Conductor: Electronic and Optical Properties from First Principles — ●MICHAEL SEIFERT, CLAUDIA RÖDL, and SILVANA BOTTI — Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany

The lack of viable *p*-type transparent conductors represents a critical bottleneck for future transparent electronics. CuI, with its direct band gap of 3.1 eV and its demonstrated *p*-type conductivity, is a promising candidate for such a material. Recently, it has raised significant renewed interest due to the production of transparent conducting bipolar CuI/ZnO heterostructure diodes, its applications as hole collection layer in organic electronics, or as promising candidate for a flexible, transparent thermoelectric material. However, a detailed theoretical understanding of the optical properties of CuI is still missing.

We use density-functional theory and many-body perturbation theory to study the structural, elastic, electronic, and optical properties of CuI in the zincblende structure (also known as the room-temperature γ phase). We have calculated key quantities of its electronic structure, in particular the band gap, effective electron and hole masses, and spin-orbit-coupling induced band splittings and compare them to available experimental values. Furthermore, we explore the optical absorption properties in the vicinity of the band gap heading towards the inclusion of excitonic effects.

O 20.2 Mon 17:45 Poster F

Hybrid functionals with self-consistent density-dependent mixing — ●THORSTEN U. AULL, AHMAD W. HURAN, and MIGUEL A. L. MARQUES — Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, 06099 Halle (Saale) Germany

One of the most famous deficiencies of Kohn-Sham density functional theory is the systematic underestimation of band gaps when they are approximated as the difference between the Kohn-Sham eigenvalues of the highest occupied eigenstate and the lowest unoccupied one [1]. Calculations with conventional hybrid functionals result in reasonable band gaps for many materials, however, within a rather narrow window for the gap [2]. This problem is attributed and large to the fact that the mixing parameter is a constant. In the work of Marques *et al.* it was shown that a suitable system-dependent mixing parameter can be estimated as a functional of the density of the system at hand [2]. Thus, the amount of the Hartree-Fock exchange energy is by far not the same for every material. Since the derivation of their mixing parameter was done at the level of the exchange-correlation potential, we study the limits of the proposed mixing parameter and show the requirements for self-consistent calculations using such an approach to gain access to energetic properties.

[1] J. Perdew, *Int. J. Quantum Chem.* **28**, 497 (1985).

[2] M. Marques *et al.*, *Phys. Rev. B* **83**, 035119 (2011).

O 20.3 Mon 17:45 Poster F

Analysis of defect states in MoSe₂ and unfolding of defect band structure — ●STEFAN ROST, CHRISTOPH FRIEDRICH, IRENE AGUILERA, BEATA KARDYNAL, and STEFAN BLÜGEL — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

We identify possible dopants in MoSe₂ that could facilitate single photon emission reflecting the symmetry of the host lattice. In particular, we investigate dopants in the chalcogen layer, because these are easiest to implant and introduce only little strain on the crystal structure. Suitable dopants are identified by density-functional-theory (DFT) studies of structural relaxation, projected density-of-states, band structure, and electron energy loss spectra, all calculated with the Jülich FLAPW code family. Calculations for the doped systems are performed using a super-cell that contains 3×3 monolayer MoSe₂ unit cells. Due to the breaking of translational symmetry, it is difficult to interpret the band structure of defect systems, in particular, for low doping concentrations. Therefore, we implemented a method for unfolding the bands in the Fleur code (www.flapw.de). The resulting band structure resembles the one of the pristine material, but it contains additional information about the defect states and their interaction with the MoSe₂ bands. It is shown that doping with group-5 and group-7 elements is promising. To understand the many-body ef-

fects on the defect level, *GW* corrections are calculated.

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O 20.4 Mon 17:45 Poster F

Electronic and Optical Properties of Pb and Sn Based Halide Perovskites from First Principles — ●CECILIA VONA¹, DMITRII NABOK¹, and CLAUDIA DRAXL^{1,2} — ¹Institut für Physik and IRIS Adlershof, Humboldt-Universität zu Berlin, Berlin, Germany — ²European Theoretical Spectroscopic Facility (ETSF)

Organic - inorganic metal halide perovskites have emerged as promising materials for next generation solar cells. However, the compounds with optimal light-harvesting properties contain lead. Therefore, a non-toxic metal that can replace Pb, without drastically decreasing the devices performance, needs to be found. Sn-based perovskites are studied as possible candidates, but their properties are not comparable with the Pb-based counterpart. To understand the different behavior of these materials, we analyze and compare their electronic and optical properties by performing first-principles calculations with the all-electron full potential code **exciting**. The electronic properties are computed in the density-functional-theory framework. The impact of different exchange-correlation functionals is investigated, and particular attention is paid to the effect of spin-orbit coupling. To get insight into the origin of the observed optical excitations, including excitonic effects, we compute the absorption spectra of Pb- and Sn-based perovskites by solving the Bethe-Salpeter equation.

O 20.5 Mon 17:45 Poster F

Towards efficient *GW* calculations in magnetic systems — ●MASOUD MANSOURI^{1,2}, PETER KOVAL^{1,2}, and DANIEL SANCHEZ-PORTAL^{1,2} — ¹Donostia International Physics Center (DIPC) — ²Centro de Física de Materiales, Centro Mixto CSIC-UPV/EHU, Paseo Manuel de Lardizabal 5, 20018 Donostia-San Sebastián, Spain

Hedin’s *GW* approximation GWA has gained popularity in the material science community because of its high quality and relatively low computational cost. A prerequisite to describe magnetic materials is the capability to describe systems containing unpaired electrons. However, spin-resolved *GW* calculations for electronic systems with unpaired electrons have not yet been extensively developed.

In this work, we benchmark unrestricted GWA for open-shell molecules. We perform one-shot G_0W_0 calculations for 42 small molecules belonging to the G2/97 test set. As reference we use the Gold standard of quantum chemistry, namely coupled cluster singles, doubles, and perturbative triples. Both reference CCSD(T) and *GW* calculations are performed using Dunning’s correlation-consistent basis sets expanded in terms of Gaussian functions. This benchmarking indicates deviations smaller than 0.5 eV, which is comparable to those found for closed-shell molecules. Furthermore, we do not find a clear connection between the spin contamination and this deviation. The results are encouraging for the use of Hedin’s GWA for magnetic materials in combination with basis sets of atomic orbitals.

O 20.6 Mon 17:45 Poster F

CO Oxidation by noble metal single atom catalysts on transition metal doped oxides — ●DEBOLINA MISRA and SATYESH YADAV — Department of Metallurgical and Materials Engineering, Indian Institute of Technology Madras, Chennai, India

Stability of transition metal (TM) defects in BaO and MgO have been studied using density functional theory. Our defect formation energy calculations show that TM atoms at various charge states can be stabilized not only at the substitutional sites, but some of them can also be accommodated well in the tetrahedral voids available in the oxides. We use this result to solve the problem of binding noble metal atoms in heterogeneous catalysis by proposing a new and effective way to anchor them on the support material. Single atoms of Pt, Pd and Au are considered on TM (Nb, Mo) doped BaO {001} surface for CO oxidation. Both hollow (H) and O-top (O) positions of the oxide surface are considered as the possible binding sites for the metal atoms. Our results reveal that compared to bare BaO {001} surface, noble metals bind more strongly when the surface is doped by Nb or Mo. For example, binding energy of Au changes from -1.28 eV (H) and -1.85 eV (O) in BaO {001}, to (i) -3.61 eV (H) and -3.69 eV (O) in Nb-doped,

and (ii) -3.57 eV (H) and -3.70 eV (O) in Mo-doped {001} surface. This is attributed to the charge transfer between TM dopants and the noble metal atoms. Our calculated adsorption energies of CO molecule on the noble metal atoms are comparable to other catalytically active systems. We further calculate the minimum energy pathway and the reaction barriers for all the elementary steps of CO oxidation.

O 20.7 Mon 17:45 Poster F

Electronic structure of epitaxially grown topological insulator (Bi,Sb)₂Te₃ films with varying magnetic doping. —

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Topological insulators (TI) have gained great interest over the last years. In particular, the topological properties of the ternary compound (Bi,Sb)₂Te₃ can be varied via doping with magnetic impurities. The magnetic doping of TI thin films is especially interesting, due to the formation of a ferromagnetic ground state, which leads to the arising of the quantum anomalous Hall state at low temperatures.

In this work we explore the electronic structure of (Bi,Sb)₂Te₃ films grown on BaF₂ (111) by angle-resolved photoelectron spectroscopy (ARPES) experiments. The nearly perfect lattice match between film and substrate results in homogenous films and ARPES data of high quality. Besides results on pristine thin films we will also present measurements on (Bi,Sb)₂Te₃ layers doped with magnetic impurities, for which an exchange splitting of the topological surface state is expected in the ferromagnetic state.

O 20.8 Mon 17:45 Poster F

Observation of surface and bulk charge density waves in LaTe₃ —

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LaTe₃ is a model Charge Density Wave (CDW) material of the rare-earth tritelluride family, with an anisotropic CDW that has a transition temperature higher than 450 K [1]. The layered structure is furthermore anisotropic, resulting in a CDW that is preferentially one dimensional: A large bandgap of 0.4 eV exists along one direction, but at the same time metallic states are present in the perpendicular direction even below the CDW transition temperature [2].

The spectral function of this material has been measured by angle resolved photoelectron spectroscopy (ARPES), including the k_{\perp} dispersion, giving access to the full 3-dimensional band structure.

In this experimental ARPES study, we show how the CDW can be largely accounted for by nesting of wave vectors at the Fermi surface.

[1] N. Ru *et al.*, Phys. Rev. B **77**, 035114 (2008)

[2] V. Brouet *et al.*, Phys. Rev. B **77**, 235104 (2008)

O 20.9 Mon 17:45 Poster F

Optimization of a numerical integration procedure for the Korrington-Kohn-Rostoker Green's function method —

•IRINA HEINZ, ALEXANDER FABIAN, PHILIPP RISIUS, and CHRISTIAN HEILIGER — Institut für theoretische Physik, Justus-Liebig-Universität Gießen, Gießen

For the description of material properties an efficient calculation of the

density of states and charge density is invaluable. We calculate these quantities based on density functional theory (DFT) within the framework of the Korrington-Kohn-Rostoker (KKR) Green's function method. This method requires integrating the Green's function within a certain energy interval. However, due to the strongly structured Green's function the numerical integration requires a lot of computational effort. Therefore, integration is typically performed in the complex energy plane.

In the present case, we consider a rectangular contour in the complex energy plane. The numerical effort required depends on the position along the contour, particularly the imaginary part of the complex energy. In order to obtain reasonable numerical accuracy in conjunction with affordable computational time, we thoroughly analyze the dependence of the integral on certain numerical parameters such as the density of the k-mesh in reciprocal space and the choice of the energy grid along the integration contour.

O 20.10 Mon 17:45 Poster F

Calculation of non-equilibrium occupation function —

•JONAS FEY, JONAS F. SCHÄFER, ALEXANDER FABIAN, PHILIPP RISIUS, MICHAEL CZERNER, and CHRISTIAN HEILIGER — Institut für theoretische Physik, Justus-Liebig-Universität Gießen, Heinrich-Buff-Ring 16, 35392 Gießen

The development of new nanoscale devices requires a precise theoretical description. This can be realized within the Keldysh formalism by means of non-equilibrium Green's functions. In order to increase the accuracy or number of these calculations the numerical effort should be kept as low as possible. In the case that the occupation function of the system is known the numerical effort can be decreased by allowing the energy to take complex values and using the residue theorem to calculate an occurring integral along paths in the complex energy plane. This is for example the case for equilibrium systems. We were able to show that for a simple model system this trick can be extended to non-equilibrium. By applying the Keldysh formalism to complex valued energies one obtains an equation to calculate the occupation function. The effects of this method on the numerical effort were examined depending on the desired accuracy.

O 20.11 Mon 17:45 Poster F

Revealing the role of the interface in the high-temperature superconductivity of single-layer FeSe/SrTiO₃ —

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Interface hosts unexpected physics due to competing orders, charge transfer, strain and other degrees of freedom for quantum interactions. At the interface between monolayer FeSe films and SrTiO₃, the superconducting transition temperature (T_c) is unexpectedly high. The mechanism for the T_c enhancement has been the central question, as it may present a new strategy for seeking out higher T_c materials. In this talk, I will introduce the series of our work on the FeSe/oxide interface involving electronic structure studies using in-situ ARPES, atomic-scale structural studies using STEM and synchrotron SXRD, and interface atomic-scale engineering using oxide MBE and MBE. We systematically reveal the relationship between superconductivity and various interfacial interactions, including strain, thickness, carrier doping, interfacial phonon energy, and interfacial electron-phonon coupling strength. Striking evidence is observed that the high T_c in FeSe/SrTiO₃ is the cooperative effect of the intrinsic pairing mechanism in the FeSe and interactions between the FeSe electrons and SrTiO₃ phonons. Moreover, we enhanced the superconducting pairing temperature of single-layer FeSe to 75K, which is a new record of pairing temperature for Fe-based superconductors and monolayer-thick films. Our results point to the promising prospect that similar cooperation of Cooper pairing channels may be a general framework to understand and design high-temperature superconductors.