TT 82: Electronic Structure Theory: General, Method Development (organized by O)

Time: Wednesday 18:15–21:00 Location: Poster A

TT 82.1 Wed 18:15 Poster A

Electron-phonon coupling in the KKR formalism — •Carsten Eberhard Mahr, Christian Franz, Marcel Giar, 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 adding a Fröhlich-type interaction to the Kohn-Sham Hamiltonian which corresponds to the previously calculated Green's function G_{ee} containing the electron-electron interaction in e.g. local density approximation (LDA), we can compute the dressed propagator through Dyson's equation as $G = G_{\mathrm{ee}} + G_{\mathrm{ee}} \cdot \Sigma_{\mathrm{eph}} \cdot G$. The self-energy Σ_{eph} is treated in Self-Consistent First Born Approximation (SCFBA), which may be obtained using a perturbative diagrammatic approach within Keldysh NEGF formalism.

We give transformed representations of the beforementioned relations and quantities for bulk calculations in the KKR 'basis' set. Based thereupon, central formulas for non-equilibrium transport in our calculational scheme are presented.

TT 82.2 Wed 18:15 Poster A

SEMT: An Orthogonal and Localized Basis-Set for All-electron Density Functional Theory — •Andrea Nobile and Stefan Blügel — Peter Grünberg Institute (PGI-1) and Institute for Advanced Simulation (IAS-1), Forschungszentrum Jülich GmbH and JARA, Jülich, Germany

Employing all-electron methods for simulations by density functional theory (DFT) allows for unbiased, highly accurate solutions of the Kohn-Sham equations. Current popular all-electron schemes like FLAPW+LO and APW+LO use a basis set that is not localized in real space and as a consequence the resulting Hamiltonian is dense. These basis sets are non-orthogonal thereby posing constraints on the choice of the eigensolver and on the usage and development of alternative, less than cubic scaling convergence schemes.

We tackle the localization and orthogonality problem by combining spectral elements with muffin-tin spheres. The introduced method, that we call spectral-element-muffin-tin (SEMT), produces a basis set that is localized and numerically orthogonal by construction.

When compared to pure spectral element methods, our basis needs a substantially smaller number of degrees of freedom per atom. The strength of the SEMT method is in the combination of all-electron, real space, sparsity and orthogonality. We demonstrate the method with our implementation (Velvet) on some elemental materials by comparing the results with FLAPW+LO calculations.

TT 82.3 Wed 18:15 Poster A

Electron-phonon relaxation times from first principle calculations — •Florian Rittweger[1,2], Nicki F. Hinsche[1], and Ingrid Mertig[1,2] — [1]Martin-Luther-Universität, Institut für Physik, Von-Seckendorff-Platz 1, DE-06120 Halle — [2]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, DE-06120 Halle

Electron-phonon interaction (EPI) is usually related to the phenomenon of superconductivity. Besides these studies the influence of the EPI on transport properties became popular in the last years.

While ARPES measurements offer experimental access to the EPI, theoretical approaches are based on the calculation of the electron-phonon matrix elements. The latter leads either to the calculation of the complex electron-phonon self-energy and therefore the renormalization of the electronic band structure or to the estimation of the electron-phonon coupling strength λ and the state-dependent relaxation time $\tau_{\mathbf{k}}$. The k-dependence of τ enters the Boltzmann equation for the computation of transport properties like the electrical conductivity, thermal conductivity and the thermopower beyond the relaxation time approximation typically used.

We calculate the EPI using linear response density functional perturbation theory and present first results and discussions for simple metals.

TT 82.4 Wed 18:15 Poster A

How Molecules Interact Through Nanostructures — •Mausumi Chattopadhyaya and Alexandre Tkatchenko — Fritz Haber Institut der MPG, Berlin, Germany

Molecules often interact and assemble in the presence of environments, such as solvents, surfaces, or nanostructures. While in the gas phase intermolecular interactions are fairly well understood, much less is known about intermolecular interactions in polarizable environments. To shed some light into this matter, we have investigated the interaction between aromatic molecules through a range of nanostructures, including graphene, h-BN, fullerenes, carbon nanotubes, and phosphorene. In each of these cases, we have computed the non-additive interaction terms by using density-functional theory with many-body dispersion interactions (DFT+MBD method [1,2]). We found that in most of the cases the intermolecular interaction energy decreases due to the presence of a nanostructure, as expected from classical electrodynamics. However, for sufficiently polarizable nanostructures, we observe a regime in which the interaction energy increases due to non-trivial quantum-mechanical fluctuations of electric dipoles. [1] Phys. Rev. Lett. 108, 236402 (2012); [2] J. Chem. Phys. 140, 18A508 (2014).

TT 82.5 Wed 18:15 Poster A

Precise dynamical response functions in all-electron methods: application to the RPA correlation energy — Markus Betzinger, •Christoph Friedrich, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, Germany

The main obstacle in calculating dynamical response functions in practice is their slow convergence with respect to the basis-set size and the number of unoccupied bands. We showed in Refs. [1,2] for the static Kohn-Sham (KS) density response in the all-electron FLAPW method that an incomplete-basis-set correction (IBC) gives rise to a much better convergence behavior. The IBC contains a basis response term that provides response contributions that lie outside the Hilbert space spanned by the original basis. These contributions, therefore, incorporate to some extent an infinite number of states. We present an extension of the IBC to the frequency domain and demonstrate that precise RPA response functions can be obtained already with small basis-set sizes and few numbers of unoccupied states. As an example, we apply the correction to the RPA correlation energy of KS density-functional theory, whose central ingredient is the RPA response function.

[1] M. Betzinger *et al.*, Phys. Rev. B **85**, 245124 (2012).

[2] M. Betzinger *et al.*, Phys. Rev. B **88**, 075130 (2013).

TT 82.6 Wed 18:15 Poster A

RPA spectra from a combination of tetrahedron method and Wannier interpolation — •Johannes Kirchmair, Christoph Friedrich, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

The polarization function within the random-phase approximation (RPA) describes the response of the electron density due to perturbations of the effective potential and is one of the key quantities in many-body perturbation theory. For example, it is employed in the calculations of GW quasiparticle energies, the RPA correlation energy, the Hubbard U parameter, but also in phonon calculations. Very often, practical calculations of the polarization function suffer from severe convergence problems. The convergence with respect to unoccupied states has recently been discussed a lot in literature and correction schemes have been proposed. Another problem is the summation over, in principle, infinitely many k points. The standard method, the so-called tetrahedron method, uses a geometrical interpolation in the three dimensions of reciprocal space that can be understood as the analog of linear interpolation in one dimension. This fast and reliable method, however, shows slow convergence of the spectral properties especially for small frequencies. In this work, we propose to take these low-energy virtual excitations from a Wannier-interpolated band structure. The Wannier interpolation is seamlessly combined with the tetrahedron method, which then takes care of the high-energy virtual excitations. We show test calculations and first results for RPA spectra.

TT 82.7 Wed 18:15 Poster A

Calculation of electron energy loss spectra for resistive switching oxides from first principles — •Roman Kováčik[1,2] and Marjana Ležaić[2] — [1]I. Physikalisches Institut, RWTH Aachen and JARA, 52056 Aachen, Germany — [2]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Calculation of the energy-loss near-edge structure (ELNES) of electron energy loss spectra (EELS) is implemented within the density functional theory framework using the full potential linearized augmented planewave (FLAPW) approach in the FLEUR code (`www.flapw.de`). The double differential cross-section is evaluated using the full relativistic treatment of incoming electrons and the transition matrix elements allowing arbitrary transitions (beyond the dipole approximation) following the formalism of Jorissen (PhD thesis, 2007). We present ELNES calculations of EELS on complex oxides with a promising application in resistive switching, such as Sr-rich phases in $SrTiO_3$.

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