MM 25: Topical Session Electron Theory II

Time: Wednesday 14:30–15:30 Location: IFW A

Topical Talk MM 25.1 Wed 14:30 IFW A

The LDA+DMFT approach to the electron theory of strongly correlated metals — •Frank Lechermann — I. Institut für Theoretische Physik, Universität Hamburg

A better understanding of the physics of realistic strongly correlated electron systems in the metallic state is one of the key ingredients in order to describe a wide range of novel solid state compounds. The complex competition between the localized and the itinerant character of interacting electrons in a manifestly multi-orbital scenario within a given (anisotropic) crystal structure is giving rise to highly interesting phenomena, such as, e.g., intricate magnetic behavior. By combining the dynamical mean-field theory (DMFT) with the local-density approximation (LDA) to density functional theory, a powerful many-body technique is established to tackle the given problem on a truly realistic level. Here the basics and the current status of the LDA+DMFT method as well as its possible future in the context of generic first-principles approaches beyond the realm of conventional exchange-correlation functionals will be discussed. On a technical level, the emphasis will be on the currently relevant interfacing steps between the Kohn-Sham band picture and the DMFT many-body representation. Results of selected materials studies will provide an insight into the high capability of the outlined framework.

MM 25.2 Wed 15:00 IFW A

Transferable tight binding description of the Fe-C interaction — •Nicholas Hatcher, Georg K. H. Madsen, and Ralf Drautz — ICAMS, Ruhr-Universität Bochum, Stiepeler Strasse 129, 44801 Bochum, Germany

A coherent transferable tight-binding (TB) parameterization of charge transfer and electronic potentials has yet to be developed for the Fe-C interaction. Additionally, while interatomic potentials have been obtained for this interaction, recent findings show that the results from these potentials are inconsistent with DFT calculations and do not give an accurate portrayal of chemical bonding in the system. Using dual DFT grid and LCAO calculations within GPAW, we obtain one electron wave functions expanded in a multiple-ζ LCAO basis. This is down-folded onto a optimal minimal basis, giving a continuous and transferable description of Fe-C bonding. By constructing a TB energy functional using these bond integrals and a parameterized interatomic repulsion, we show how an accurate description of the energy hierarchy of relevant Fe-C structures, including the interstitial occupancy of carbon in iron, can be achieved. This simple model based on physical insights may be used to study systems containing thousands of atoms.

MM 25.3 Wed 15:15 IFW A

Charge transfer and localization within a tight binding framework — •Georg K. H. Madsen, Eunan J. McEniry, Nick Hatcher, and Ralf Drautz — ICAMS, Ruhr-Universität Bochum, Stiepeler Strasse 129, 44801 Bochum, Germany

The computational cost of density functional theory (DFT) places limitations on its application to both extended defects and to sampling the configuration space of complex phases. While these problems can be treated by empirical potentials, these can be questioned both from a view of transferability and physical justification.

From a computational point of view and from the wish to gain physical insight, one successful intermediate method between DFT and empirical potentials is the tight-binding (TB) method. In its conventional form the TB method models the total energy as a repulsive pair potential and a bonding many-body term. Using a down-folding technique we demonstrate how TB parameterizations can be constructed which involve a minimum number of fitting parameters and are based as closely as possible on the DFT energy functional.

We will discuss transition metal oxides and long range charge transfer within a tight binding framework based on the second order expansion of the DFT energy functional.