Dynamical mean field theory studies of the rare earth hexaboride compounds

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In Short

- Investigate spectral properties of rare earth hexaboride compounds, which are strongly correlated materials with unconventional behavior.
- Implement and apply a combined approach using Density Functional Theory (DFT) and Dynamical Mean Field Theory (DMFT) for a realistic modeling of these materials.
- Large scale computations using the continuous-time hybridization expansion quantum Monte Carlo algorithm (CT-HYB) in order to be able to perform the DFT+DMFT approach.

Strongly correlated materials are an important field of research in modern solid state physics. These materials show a diversity of unconventional phenomena [1], including high-temperature superconductivity, colossal magnetoresistance and heavy fermion physics, that are useful for technical applications. A material is called strongly correlated, if electron-electron interactions determine its properties. This can lead to unconventionally ordered ground states or exotic phases like non-Fermi liquids, which exhibit anomalous transport properties in contrast to systems, in which correlation effects can be neglected. Incompletely filled atomic d- or f-shells are typical for a material exhibiting strongly correlated electron effects [1]. The localization of the f-electrons in rare earth ions is even stronger than the localization of d-electrons in transition metals, which leads to a large Coulomb interaction and thus to strong correlation effects.

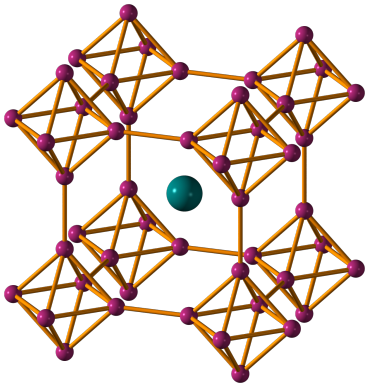

***Figure 1:** Structure of the rare earth hexaborides. The rare earth atom (teal) sits at the center of a cubic cage of boron (magenta) octahedra located at the corners of the cube.*

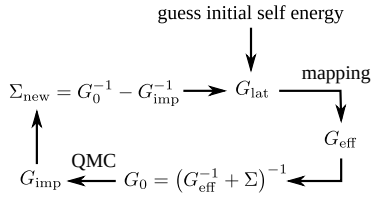

***Figure 2:** So-called DMFT cycle for the computation of the self-energy Σ and the system's Green's function $G_{\rm lat}$, which is at the heart of our numerical simulations for a more realistic modeling of the rare-earth hexaboride compounds. The numerically most expensive part is the QMC (Quantum Monte Carlo) step, which we plan to perform on the HPC environment at HLRN.*

In this project, we examine the properties of rare earth hexaborides, which are depicted in Fig. 1. A starting point for our study is that correlation effects lead to unconventional signatures in photoemission experiments [2], which are lacking a theoretical understanding so far. To approach this phenomenon, we apply large scale numerical methods. In particular, we combine Density Functional Theory (DFT) with Dynamical Mean Field Theory (DMFT), which gives the opportunity for a more realistic modelling of materials. In Fig. 2 we depict the DMFT approach in a sketch showing the so-called DMFT-cycle. In this approach, the numerically most demanding part is the Quantum Monte Carlo (QMC) step. For this, it is important to get access to large scale computing facilities like HLRN. Having access to these computational resources allows us to compute properties at low temperatures relevant for the experiments, and allows us to also take into account more effects, like spin-orbit coupling, many orbitals and the full Coulomb interaction tensor. Our simulations at HLRN will therefore help us to investigate fundamental properties of these materials like superconductivity, Kondo behavior and ordering phenomena at low temperatures.

WWW

http://www.theorie.physik.uni-goettingen.de/forschung

More Information

[1] A. Georges, L. de' Medici, and J. Mravlje *Annual Review of Condensed Matter Physics* **4**(1), 137 (2013). doi:10.1146/annurev-conmatphys-020911-125045

[2] S. Patil, G. Adhikary, G. Balakrishnan, and K. Maiti *J. Phys.: Condens. Matter*

23(49), 495601 (2011). doi:10.1088/0953-8984/23/49/495601

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