Insights into the correlations of the iron-based superconductors from DFT+DMFT calculations

Markus Aichhorn

Centre de Physique Thorique (CPHT), cole Polytechnique Palaiseau

Since the discovery of the iron-based high-temperature superconductors with superconducting Tc of up to roughly 50 Kelvin, it has been a long-standing debate if correlations play an important role in these compounds. In order to investigate this question we use a combination of ab-initio (Density-Functional Theory) methods and many-body techniques that can account for correlations beyond DFT. The methods of choice for this purpose are the full-potential linearized augmented plane wave technique as implemented in the Wien2K package, and for dealing with the correlations we apply the Dynamical Mean-Field Theory (DMFT). Using the continuous-time Quantum Monte-Carlo (CTQMC) technique that has been developed in recent years, we can address relevant temperatures (room temperature and even below), and also arbitray interaction regimes.

Using our approach for the parent compound LaOFeAs of the 1111 family of the iron Pnictides, we can show that this system is in a moderately correlated regime, with a quasi-particle weight of about Z=0.5 to 0.6, when reasonable interaction parameters for the Coulomb interaction U and Hunds exchange J are used. Furthermore, this result is quite robust on the number of Kohn-Sham bands used for constructing the Wannier functions for the DMFT calculation. We also checked that the inclusion/neglect of the so-called spin-flip and pair-hopping terms in the Hunds-rule exchange cannot change these results to give a strongly-correlated material.