Electronic structure calculations for correlated materials – A Dynamical Mean Field Theory perspective

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Dynamical mean field theory (DMFT), in conjunction with electronic structure techniques such as density functional theory (DFT), has led to tremendous progress in the description of excited state properties of materials with strong electronic Coulomb correlations. The challenge nowadays consists in refining the interface of electronic structure and many-body theory in order to develop quantitatively accurate predictive schemes.

We review in particular recent efforts of incorporating dynamical screening effects into a DMFT-based description of correlated materials [1]. Such effects can stem either from higher energy degrees of freedom that have been integrated out [2] or from nonlocal processes that are effectively backfolded into a local description. This can be conveniently done by combined many-body perturbation theory and dynamical mean field theory ("GW+DMFT") techniques [3]. An analysis of the effects of the different corrections to standard DFT+DMFT schemes leads to new insights also into DFT itself [4, 5].

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