Dynamical mean field theory extended to nano-scopic systems and molecules

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Abstract:

Quantum mechanics and its relation to material design and energy needs are important for almost every branch of the industry. Density functional theory (DFT) was successful at making accurate predictions for many materials, in particular compounds which have a metallic behaviour. DFT combines high accuracy and moderate computational cost, but the computational effort of performing calculations with conventional DFT approaches is still non negligible and scales with the cube of the number of atoms.
A recent optimised implementation of DFT was however shown to scale linearly with the number of atoms (ONETEP), and opened the route to large scale DFT calculations for molecules and nanoscopic systems.

Nonetheless, one bottleneck of DFT and ONETEP, is that it fails at describing well some of the compounds where strong correlations are present, in particular because the computational scheme has to capture both the band-like character of the uncorrelated part of the compound and the Mott-like features emerging from the local strongly correlated centres. A recent progress has been made in this direction by the dynamical mean-field theory (DMFT), that allows to describe the two limits (metal and insulator) in a remarkable precise way when combined with DFT.

Recently, the TOSCAM package (TO-lbox for S-trongly C-orrelated A-pproaches to M-olecules), a DMFT implementation for ONETEP, allowed to expand the scope of DMFT to nanoscopic systems and molecules, and provides a new method bridging the fields of Physics and quantum Chemistry.
The method will be discussed and illustrated by a few case of studies (ligand binding in Myoglobin and Haemoglobin).

References :

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