Many-body effects in oxygen transport proteins: a dynamical mean-field theory study

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Title:

Abstract:

Phenomena that are connected to quantum mechanics, such as magnetism, transport, and the effect of impurity atoms and disorder, and their 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 nano-structures. 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 boththe band-like character of the uncorrelated part of the compound and the Mott-like features emerging from the local strongly correlated atoms. 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. The ONETEP+DMFT implementation and strategies to overcome the main bottlenecks of this type of calculations will be discussed, and its applications on oxygen transport proteins, e.g. Haemoglobin and Hemocyanin, will be demonstrated. The role of many body effects for the binding of transition metal complexes will be discussed.

References :

PRL 108, 256402 ' 12
PRL 110, 106402 ' 13
PNAS 111, 5790 '14