Dynamical Mean Field Theory as an alternative to the traditional methods for treating extended systems

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In quantum chemistry, calculations for strongly correlated solids are impossible besides the smallest cases because of a prohibitive cost of the explicit treatment of periodic boundary conditions. However, in condensed matter physics, Dynamical Mean Field Theory (DMFT), which is an established method, enables the treatment of solids without explicitly imposing periodic boundary condition. The success of DMFT is based on a self-consistency cycle that takes into account the mutual interaction between a unit cell and the environment. Consequently, one of the most important steps in DMFT is the solution of a Hamiltonian that describes the unit cell and its simplified interaction with the surrounding orbitals. Because of the "frequency" dependence of the embedding DMFT includes significant correlation effects that go beyond the simpler QM/QM approaches so far used in quantum chemistry. In order to solve such a Hamiltonian, one can use any existing quantum chemistry method that allows us to treat strongly correlated electrons. Such a treatment makes possible calculations for strongly correlated solids. Thus, a hierarchy of methods similar to the one existing for treatment of molecules (MBPT2, CCSD, MRCI, DMRG) can be established for the treatment of strongly correlated solids within the DMFT framework. I will introduce our recent contributions in adapting the Dynamical Mean Field Theory (DMFT) to realistic quantum chemical calculations for solids, and I will show applications to the hydrogen solid, fcc-nickel, and to the problem of a cobalt atom deposited on a copper (111) surface. Finally, I will discuss how the DMFT embedding theory can be adjusted to treat molecular systems.