Towards an efficient mean-field wave-function based theory for periodic systems

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In this poster, we present an efficient implementation of a mean-field theory including exact exchange for periodic systems using Gaussian basis functions. These atom-centred orbitals make use of the local nature of electron densities around the atomic sites, and as a result, are more suitable than plane waves for the study of defects, low dimensional systems, and local correlation. Our implementation utilises density fitting as well as the fast multipole method (FMM) to achieve maximal efficiency in the construction of the Fock matrix. Evaluation of the long-range Coulomb interactions is done in the spirit of a renormalization method[1] and Ewald[2] summation method. This work provides the basis for a reliable and systematically improvable framework for strongly correlated extended systems via embedding methods such as dynamical mean-field theory (DMFT)[3], density matrix embedding theory (DMET)[4], or wave function in density functional theory (DFT) embedding[5].

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