In the field of computational materials science, explicit wavefunction expansions (with some notable exceptions) are generally avoided as the central quantum variable, despite certain formal advantages in terms of accuracy and improvability. The biggest impediment to their use in computational electronic structure in the solid state is the slow convergence with supercell size required to reach the thermodynamic limit and converge finite size effects. Here, we discuss a new method, Density Matrix Embedding Theory, which aims to rigorously map the infinite bulk system onto a finite quantum model which can be readily solved with quantum chemical techniques. Obvious similarities with the Dynamical Mean Field Theory formalism will be discussed, but key differences will also be highlighted, before demonstrating the simple approach for a range of static and dynamic properties of strongly correlated systems.

References:

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