Accurate Embedding Methods for Excited States

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Density-based embedding methods have found a widespread use in electronic-structure theory over the past years [1]. Among the most challenging applications with such embedding methods are calculations of excited electronic states in complex environments by means of wavefunction-in-DFT embedding. In this talk, our recent efforts towards fully consistent state-specific embedding potentials for such applications will be discussed [2, 3]. In particular, the choice of the wavefunction method (CASPT2, CC, QMC) and the dependence of the embedding potentials on the excited-state density of the embedded system will be discussed. Pilot results from a fully consistent DMRG-in-DFT implementation will be presented [4], and conceptual questions in the context of wavefunction-in-DFT embedding for excited states will be discussed [5].

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