Density Matrix Embedding Theory Based Multi-Configurational Wavefunction Approach to Strongly Correlated Single-Impurity Systems

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Abstract: Electronic structure theory for strongly correlated systems (SCSs) poses a long-standing challenge in quantum chemistry and has attracted tremendous efforts in recent decades. Among various theoretical methods that have been developed for strongly correlated molecular systems, multi-configurational self-consistent field (MCSCF) theory has played a particularly important role as it provides a systematic approach to static correlation, which is the most challenging part of SCSs. However, due to the exponential scaling of MCSCF-type methods with respect to the size of the system under study, a direct application of those approaches to complex systems is computationally demanding and becomes even prohibitive for extended systems like solids and surfaces. Density matrix embedding theory (DMET), which combines low-level (e.g., Hartree-Fock approximation) and high-level correlated quantum chemistry methods, provides a systematic framework to reduce the computational cost for treating SCSs. In this work, we present an efficient quantum embedding approach that combines DMET with the complete active space self-consistent field and subsequent state interaction treatment of spin–orbit coupling (CASSI-SO) and apply it to an efficient ab initio study of strongly correlated single-impurity systems.