Model Hamiltonians for iron-sulfur cluster complexes using Density Matrix Downfolding and Density Matrix Renormalization Group

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Density Matrix Downfolding (DMD) is a recently introduced method to obtain optimally parametrized effective Hamiltonians. The DMD theory establishes that the optimal effective Hamiltonian in a defined low-energy space is obtained by matching the exact and effective energy functionals in such a way that the two spaces have the same spectrum. The exact low-energy spectrum is approximated by high-level ab initio calculations and fitted to the effective model by least squares minimization after a rigorous process of assessing the data points. DMD is easily implementable and applicable, but its use has been restricted to the field of condensed-matter physics. This work explored the applicability of DMD to a number of model chemical systems, focusing on iron-sulfur cluster complexes, which model the active sites of some enzymes that are responsible for many essential metabolic pathways in living organisms. The Density Matrix Renormalization Group (DMRG) method is used to generate a number of states that belong to the low-energy space of each system. The preliminary results show that DMD provides a reliable and computationally inexpensive way of obtaining effective Hamiltonians, which can, in turn, be used to build models on the catalytic behavior of enzymes and to perform quantum dynamical reactivity simulations.