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Embedding methods: application and development JIN CHENG, Chemistry Department, Princeton University, FLORIAN LIBISCH, EMILY CARTER, Department of Mechanical and Aerospace Engineering, Princeton University — Correlated-wavefunction/density functional theory (CW/DFT) embedding methods aim to combine the formally exact correlation treatment in CW methods with the high efficiency of DFT. By partitioning a system into a cluster and its environment, each part can be treated independently. Different embedding schemes have been proposed. The density-based scheme searches for a global embedding potential mediating the interaction on the DFT level. The potential can then be used in CW calculations, e.g., to investigate hot-electron assisted H_2 dissociation on Al and Au surfaces. Experimentally, optical excitations of plasmons efficiently create the required hot electrons. The embedded CW calculations validates that the hot electrons play a key role. However, this method neglects the back-action of the cluster on the environment. To solve this problem, a potential-based scheme has been proposed [*J. Chem. Phys.*, 135, 194104 (2011)] that allows for a self-consistent combination of different ab-initio methods. Such an embedding potential thus goes beyond the DFT level. The heterogeneity involved poses various numerical challenges. We report on efforts to construct appropriate basis sets and pseudopotentials as well as to optimize the numerical procedure.

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