Frozen-Density Embedding Theory: first-principles based strategy for multi-level simulations

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Frozen-Density Embedding Theory (FDET) was formulated originally for embedding a Kohn-Sham system in an environment characterized exclusively by its charge density [1,2] and extended further for embedding other systems: interacting wave function [3] and one-particle density matrix [4].
The basic result of FDET is that the partial minimization of the total energy with respect to the variation localized in the embedded system can be achieved using an additional potential (orbital-free embedding potential) which is uniquely determined by the charge densities into which the total charge density is partitioned. Multi-level type of description for a complex system is achieved this by means of applying various levels of approximations for different components of the total density.

We will overview the most recent benchmarking [5] and practical applications of FDET methodology of the computational methods based on FDET in studies of excitation levels for molecules in condensed phase [6].

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