# FDE-ADC: Multiscale density embedding with an accurate wavefunction method

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In the presence of an environment, excitation energies, properties and sometimes even reactivity of the target molecule may change drastically. Thus, including environmental effects into quantum chemical calculations either by implicit or explicit models is necessary for an adequate description of these systems. Frozen-Density Embedding Theory (FDET)[1,2] provides a formal framework in which the whole system is described by means of two independent quantities: the embedded wavefunction (interacting or not) and the density associated with the environment.

The FDET approach can conveniently be combined with pertubative wavefunction methods, e.g. the Algebraic Diagrammatic Construction (ADC) scheme for the polarization propagator[3,4]. We present the new multiscale variant FDE-ADC[5] as a combination of FDET and ADC. The current implementation of FDE-ADC uses the Linearized FDET formalism[6], which in comparison to FDET, is significantly less expensive computationally and more importantly leads to self-consistency between the energy and embedding potential preserving simultaneously the orthogonality of the embedded wave functions for each electronic state.

Three molecular model systems were studied using two different FDE-ADC techniques in which the environment consisted of up to five water molecules. The molecular test systems were chosen to investigate molecule - environment interactions of varying strength from dispersion interaction up to multiple hydrogen bonds. The overall difference between the supermolecular ADC calculations and the FDE-ADC calculations in excitation energies is lower than 0.09 eV (max) and 0.032 eV in average. Also oscillator strengths are reproduced in good agreement with the supermolecular calculation. Initial results show that the FDE-ADC method is a promising approach for considering environmental effects on electronically excited states.

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