Workshops

Density-based embedding for multiscale simulations

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Visa requirements

Differential polarization effects with wave function/DFT embedding for excited states

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Abstract

I will present the approach we recently developed to extend wave function in density functional theory (WF/DFT) methods to compute the excitation energies of a molecule in a responsive environment [1]. Our scheme relies on the construction of state-specific density-based embedding potentials within a modified subsystem DFT approach. I will discuss the general expression of the ground- and excited-state energy difference of the total system, and compare some practical recipes for the construction of an approximate excited-state DFT density to polarize the environment, to the use of accurate WF densities for the active part. These concepts will be demonstrated with the computation of the state-independent and state-specific WF/DFT excitation energies of several small organic molecules using perturbative (CASPT2) and quantum Monte Carlo (QMC) methods as wave function approaches.

References

[1] C. Daday, C. Konig, O. Valsson, J. Neugebauer, and C. Filippi, J. Chem. Theory. Comput. 9, 2355 (2013).

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