Density-based embedding for multiscale simulations

March 24, 2014 to March 27, 2014

Location : CECAM-HQ-EPFL, Lausanne, Switzerland
EPFL on iPhone

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A density-division embedding potential inversion technique

Octavio Roncero

Abstract

A method is proposed to partition the density of a system in two portions. The density on each subsystem is the solution of a Fock equation modified by the addition of an "embedding" potential. This embedding potential is obtained iteratively by minimizing the difference between the electronic densities of the total system and the sum of the subsystems. Thus, the electronic density partition and the two embedding potentials, one per portion, are obtained at the same time
within the procedure, warranting the v-representability of the two densities obtained. The method is first applied to a linear H10 chain to illustrate how it works. The orbitals obtained are localized on each subsystem, and can be used to include local electronic correlation using currently available ab initio programs. Finally, the method is applied to include the electronic correlation needed to describe the van derWaals interaction between H10 chains and H2 molecules, of ca. 12 meV, giving very accurate results. Some preliminary results on the Br2-H2O will also be shown.

References

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