DENSITY FUNCTIONAL EMBEDDING SCHEME FOR MOLECULES AND PERIODIC SYSTEMS COUPLED WITH WAVE FUNCTION METHODS AND REAL TIME-TIME DEPENDENT DENSITY FUNCTIONAL THEORY

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An implementation of density functional embedding theory, within the frozen density embedding formalism [1], for molecules and periodic systems in the TURBOMOLE program package [2] using Gaussian basis functions is presented. The subsystem of interest may be described by density functional theory (DFT) or wave function theory (WFT) methods**,** while the environment density is determined using DFT. Employing an embedding potential based either on non-additive kinetic energy density functional or a level-shift projection operator [3], DFT-in-DFT or WFT-in-DFT is performed. While the embedding potential may be updated during the embedding procedure for DFT-in-DFT calculations, the WFT-in-DFT utilize a fixed embedding potential. The Coulomb contribution to the Kohn-Sham matrices of the subsystems as well as to the embedding potential is efficiently calculated using a combination of density fitting and continuous fast multipole methods [4]. The exchange-correlation and the nonadditive kinetic energy potentials are evaluated using the linear scaling hierarchical integration scheme [5].
Furthermore, the embedding scheme is coupled with a recent and highly efficient real timetime dependent DFT implementation [6] that allows for the study of the non-linear optical response of the embedded subsystem.

References

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