Coupled Cluster Studies of Molecules in Condensed Matter Environments

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Coupled cluster is a highly accurate quantum chemistry method, but the computational costs associated with coupled cluster scale poorly with the number of included electrons. Methods to reduce the required number of included electrons in such calculations [1] can help reduce the costs associated with these calculations. Through the use of external potentials from lower-level calculations, we have performed coupled cluster calculations on molecules surrounded by a variety of environments. We have implemented and tested this approach with the DALTON quantum chemistry code and the JDFTx density functional theory code. Our method is applicable to molecules in environments that can be described by potentials, with diverse applications including solvation studies and the refinement of eigenvectors of the molecular response matrix.

[1] K. Schwarz, R. Sundararaman, K. Letchworth-Weaver, T. A. Arias, and R. G. Hennig, Phys. Rev. B **85**, 201 102(R) (2012).

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