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Accurate and systematically improvable quantum embedding methods for complex systems JASON GOODPASTER, TAYLOR BARNES, California Institute of Technology, FREDERICK MANBY, University of Bristol, THOMAS MILLER, California Institute of Technology — We describe embedded density functional theory (e-DFT) methods that avoid approximations to the kinetic energy functional and provide a formally exact approach to performing electronic structure calculations in the e-DFT framework. This framework allows systems to be divided into smaller subsystems which can be treated at different levels of theory, with the intersubsystem potential calculated using our e-DFT protocol. We use this framework to develop robust wavefunction embedding methods. This allows for wavefunction calculations to be used in regions of large systems where DFT is known to perform poorly, such as van der Waals interactions and strongly correlated electrons. Through a systematic analysis of embedding errors, we determine the largest source of error from wavefunction-in-DFT embedding to be the evaluation of the approximate non-additive exchange-correlation functional. We suggest new algorithms to systematically reduce these errors. These improvements allow for embedding methods that accurately reproduce reference couple-cluster calculations for a series of chemical reactions.

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