

Abstract Submitted
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Multi-level partitioning using embedded density functional theory JASON GOODPASTER, TAYLOR BARNES, THOMAS MILLER, California Institute of Technology — Embedded density functional theory (e-DFT) methods are typically limited to the description of weakly interacting systems, because an exact form of the kinetic energy (KE) density functional is unknown. We have developed a method that avoids approximations to the KE functional and provides 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 inter-subsystem potential calculated using our e-DFT protocol. Therefore, in regions of large systems where DFT is known to perform poorly, such as van der Waals interactions and strongly correlated electrons, wavefunction calculations can be used. We discuss density partitioning strategies for embedded density functional theory and the accuracy of this multi-level method.

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