

Abstract Submitted
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**Strongly Interacting Molecular Subsystems Using DFT-in-DFT
Embedding Theory with External Orbital Orthogonality** PATRICK

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— Since most ab initio methods for molecular electronic structure are limited in applicability by polynomially increasing computational costs with system size, localization and embedding techniques are among the leading research efforts in the development of methods that can well describe large systems. Since embedding schemes naturally use a “divide and conquer” approach, they are particularly attractive. We recently introduced a new variant of DFT-in-DFT embedding theory that enforces orbital orthogonality between subsystems, thereby completely obviating the use of error-prone kinetic energy functionals; moreover, no calculation of the total system is required at any stage. Here, we present density difference maps and potential energy curves for selected strongly interacting subsystems, including complete dissociation of covalent bonds, obtained with our new embedding protocol. The electron density difference maps presented here compare densities obtained with the new embedding method, and with conventional DFT-in-DFT, to Kohn-Sham (KS)-DFT densities. It is shown that whereas conventional DFT-in-DFT leads to large density deviations, particularly at the interfaces between subsystems, the new method accurately represents the density at all points in space and leads to only negligible density deviations ($\approx 10^{-5}$ e/a₀³). To our knowledge, this new embedding method is the first variant of DFT-in-DFT to accurately dissociate actual covalent bonds.

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