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Exactly embedded DFT for the efficient simulation of large systems TAYLOR BARNES, JASON GOODPASTER, THOMAS MILLER, California Institute of Technology — Although standard wavefunction-based approaches to electronic structure problems have experienced great success in the study of small systems, their poor size scaling prohibits their application to larger systems. One promising technique for overcoming this scaling problem is embedded Density Functional Theory (e-DFT), in which a large system is divided into many smaller subsystems, with individual wavefunction-based calculations being performed on each subsystem. Using our newly developed Exactly Embedded (EE) technique, we demonstrate highly accurate e-DFT calculations on aqueous systems consisting of hundreds of atoms. Furthermore, these calculations are shown to exhibit excellent size scaling and to be massively parallelizable, allowing for efficient calculations of condensed-phase systems.

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