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**Optimized Gaussian Basis Sets for Plane-Wave Compatible Calculations** JIN CHENG, Department of chemistry, Princeton University, FLORIAN LIBISCH, MOHAN CHEN, EMILY CARTER, Department of Mechanical and Aerospace Engineering, Princeton University — The Wu-Yang optimized effective potential method (WY-OEP) is becoming widely used in embedding theories to get the exact kinetic energy potential for a given density. Our group implemented this scheme in the plane-wave code (ABINIT) and showed that it performs well for potential functional embedding on the density functional theory (DFT)/DFT level. To extend this embedding scheme and the WY-OEP method to correlated-wavefunction (CW)/DFT embedding, it is necessary to perform a WY-OEP calculation with a CW density. However, the incompleteness of Gaussian basis sets used in CW calculations causes numerical instabilities and leads to unphysical behavior in the kinetic energy potential. We propose a method to construct a basis set that systematically approaches the plane-wave basis density while retaining the quality of the CW. By doing so, basis set incompatibility has been eliminated. Test calculations show that good agreement for the density can be reached and the CW calculations give reasonable results. Furthermore, the WY-OEP has been performed with densities from a variety of CWs. The densities are well-reproduced and the kinetic energy potential is free of unphysical behavior, boding well for such potential-functional-embedded CW calculations.

Jin Cheng  
Department of chemistry, Princeton University

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