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Iterative Optimized Effective Potential and Exact Exchange Calculations at Finite Temperature N.A. MODINE, Sandia National Laboratories, R.A. LIPPERT, MIT Department of Mathematics, A.F. WRIGHT, R.P. MULLER, M.P. SEARS, A.E. MATTSSON, M.P. DESJARLAIS, Sandia National Laboratories
— We report the implementation of an iterative scheme for calculating the Optimized Effective Potential (OEP). Given an energy functional that depends explicitly on the Kohn-Sham wave functions, and therefore, implicitly on the local effective potential appearing in the Kohn-Sham equations, a gradient-based minimization is used to find the potential that minimizes the energy. Previous work has shown how to find the gradient of such an energy with respect to the effective potential in the zero-temperature limit. We discuss a density-matrix-based derivation of the gradient that generalizes the previous results to the finite temperature regime, and we describe important optimizations used in our implementation. We have applied our OEP approach to the Hartree-Fock energy expression to perform Exact Exchange (EXX) calculations. We report our EXX results for common semiconductors and ordered phases of hydrogen at zero and finite electronic temperatures. We also discuss issues involved in the implementation of forces within the OEP/EXX approach.
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