Implementation of the Optimized Effective Potential and Exact Exchange in Socorro

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Given an energy functional that depends explicitly on the Kohn-Sham wave functions, and therefore, implicitly on the local potential appearing in the Kohn-Sham equations and the density, the Optimized Effective Potential (OEP) is the potential that minimizes the energy. The OEP approach allows the treatment of wave function dependent functionals within the Kohn-Sham Density Functional Theory (DFT) framework. One example of such a functional is the Hartree-Fock exchange expression, and when it is used as the exchange-correlation energy within the OEP approach, the resulting approximate DFT is known as the Exact Exchange (EXX) approximation. We report implementation of the OEP method and the EXX approximation within the Socorro electronic structure software using an iterative, gradient-based minimization to find the OEP. We discuss a density-matrix-based derivation of the necessary gradient that generalizes previous results to finite temperatures, and we describe important optimizations used in our implementation. The OEP/EXX approach should capture important physical behavior associated with the accurate treatment of the exchange interaction while allowing better performance in a plane-wave basis set compared to Hartree-Fock and hybrid functionals. We demonstrate the results of applying our software to representative systems and also discuss remaining issues within the OEP/EXX approach.

Sandia National Laboratories is a multi-program laboratory operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin company, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.