Hartree-Fock Pseudopotentials within the Opium Package

Eric J. Walter, Wissam A. Al-Saidi, and Henry Krakauer

Department of Physics, College of William and Mary
Williamsburg, VA

We report soft Hartree-Fock based pseudopotentials computed within the framework of the OPIUM pseudopotential construction package. The long range tail due to the non locality of the exchange potential is removed using a self-consistent damping mechanism as employed in exact exchange [1] and recent Hartree-Fock pseudopotentials [2]. The binding energies of several dimers computed using these pseudopotentials within a planewave Hartree-Fock code show good agreement with all-electron results. Incorporation of the Hartree-Fock method into an LDA/GGA atomic code allows for the highly accurate hybrid exchange-correlation functions (such as B3LYP) to be implemented at the pseudopotential level. Expansion of these pseudopotentials within a Gaussian basis set will also be presented.

[1] E. Engel, A. Höck, R. N. Schmid, R. M. Dreizler, and N. Chetty, Phys. Rev. B **64**, 125111 (2001).

[2] J. R. Trail and R. J. Needs, J. Chem. Phys. **122**, 014112 (2005).