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A Projector Augmented Wave Treatment of Fock Exchange in Hartree-Fock and Optimized Effective Potential Calculations[1] XIAO XU, N.A.W. HOLZWARTH, Wake Forest University — The use of orbital-dependent exchange-correlation functionals within electronic structure calculations has recently received renewed attention as a means of improving accuracy. In particular, the Fock exchange functional exactly cancels the electron self-interaction error which can be particularly significant in transition metals and other materials with localized orbitals. Since the Projector Augmented Wave (PAW) formalism[2] accurately evaluates the interaction integrals including all multiple moments, it is a natural choice for representing the Fock exchange functional within an efficient pseudopotential-like scheme. We have adapted the PAW formalism for use both in Hartree-Fock (HF) theory and in the KLI approximation to Optimized Effective Potential theory.[3] We show that the effects of core electrons are significant and can be accurately treated within a frozen core orbital approximation.[4] PAW-HF and PAW-KLI basis, projector, and pseudopotential functions are presented for several elements throughout the periodic table.

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[2]P. E. Blöchl, *Phys. Rev. B* **50**, 17953 (1994).
[3]J. B. Krieger, Y. Li and G. J. Iafrate *Phys. Rev. A* **45** 101 (1992).
[4]Xiao Xu and N. A. W. Holzwarth, *Phys. Rev. B* **81** 245105 (2010).

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