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Projector Augmented Wave formulation of orbital-dependent exchange-correlation functionals[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 for improving the accuracy of the calculations, especially correcting self-interaction errors. Since the Projector Augmented Wave (PAW) method[2] is an efficient pseudopotential-like scheme which ensures accurate evaluation of all multipole moments of direct and exchange Coulomb integrals, it is a natural choice for implementing orbital-dependent formalisms. Using Fock exchange as an example of an orbital-dependent functional, we developed the formulation and numerical implementation of the approximate optimized effective potential formalism of Kreiger, Li, and Iafrate (KLI)[3] within the PAW method, comparing results with the analogous Hartree-Fock treatment.[4] Test results are presented for ground state properties of two well-known materials – diamond and LiF. This formalism can be extended to treat orbital-dependent functionals more generally.

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[2]P. 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); **84**, 155113 (2011).

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