Abstract Submitted
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A Projector Augmented Wave Formulation of the Optimized Effective Potential Formalism[1] XIAO XU, N.A.W. HOLZWARTH, Wake Forest University — The optimized effective potential (OEP) or exact exchange (EXX) formalism has recently received renewed attention[2] as a method which can improve the accuracy of density functional calculations by representing orbital-dependent functionals and avoiding self-interaction errors found in density functionals. Since the Projector Augmented Wave (PAW) formalism[3] ensures accurate evaluation of interaction integrals by controlling the multipole moments,[4] it is a natural choice for implementing OEP within an efficient pseudopotential-like scheme. We developed a frozen core approximation scheme for the atomic all-electron OEP formalism, partitioning the exchange potential into core and valence contributions. The corresponding valence exchange pseudopotential for PAW, $\widetilde{V}_x^{\rm vale}(\mathbf{r})$, can be derived in a similar way so that for $r > R_c$, $\widetilde{V}_x^{\rm vale}(\mathbf{r}) = V_x^{\rm vale}(\mathbf{r})$. We have investigated the behavior of PAW-OEP basis, projector, and pseudopotential functions for several elements throughout the periodic table.

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[3]P. Blöchl, PRB **50**, 17953 (1994); N. A. W. Holzwarth *et al*, PRB **55**, 2005 (1997).
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