Projector Augmented Wave (PAW) Implementation of Hartree-Fock Formalism*

N. A. W. Holzwarth, and Xiao Xu

Department of Physics, Wake Forest University
Winston-Salem, NC

The PAW[1] formalism is well established as a powerful method of evaluating electronic structure with density functional (Kohn-Sham) theory. Previous work by the VASP group[2] has shown that the PAW formalism is able to accurately evaluate the Fock exchange, including all of its multipole moments. In this poster, we first compare two kinds of treatments of core electron contributions within Fock exchange, and argue that core-valence exchange interactions should be treated in terms of orbitals. From this so-called *frozen core orbital* approximation, we show how the integral-differential equations of Hartree-Fock theory can be represented within the PAW formalism.

The results section is organized as follows: I We present the numerical algorithms for Hartree Fock II We discuss the accuracy of the frozencore approximation for Hartree-Fock calculations in various atoms. This serves as a lower bound measure of frozencore error for electronic structure calculations of these elements using PAW and other electronic structure methods. III. We present the Hartree Fock PAW implementation and some representative results of atom-centered wavefunctions .

---

*This work was supported by NSF grants NSF DMR-0405456, DMR-0427055, and DMR-0705239.Computations were performed on the Wake Forest University DEAC cluster, a centrally managed resource with support provided in part by the University.

---

[1] P. E. Blöchl, Phys. Rev. B **50** 17953 (1994).

[2] J. Paier, R. Hirschl, M. Marsman, and G. Kresse, J. Chem. Phys., **122**, 234102 (2005).