A Projector Augmented Wave Treatment of Fock Exchange in Hartree-Fock and Optimized Effective Potential Calculations

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 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. We show that the effects of core electrons are significant and can be accurately treated within a frozen core orbital approximation. PAW-HF and PAW-KLI basis, projector, and pseudopotential functions are presented for several elements throughout the periodic table.

1Supported by NSF Grant DMR-0705239.