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Effects of core-valence interaction in the screened-exchange density functional method[1] BYOUNGHAK LEE, LIN-WANG WANG, Lawrence Berkeley National Lab — We present a new development for the screened-exchange (sX) density functional method using a planewave basis. In the screened-exchange density functional method, an explicit screened exchange interaction term is included in the total energy expression. When implemented with a planewave basis, the LDA derived norm-conserving pseudopotentials have usually been used without any change for the sX calculation. While this works well for valence s and p orbitals with the same quantum numbers, we found that there is a problem when d orbitals with a different quantum number are included. This is due to an error in the exchange integral between d and s, p orbitals stemming from the use of pseudowavefunctions. As a result, the calculated bulk electronic structures have much smaller band gaps compared to all electron sX calculations and experiments. We propose a scheme to correct the d-s/p exchange integrals using atomic orbital projection operators. We test our scheme on ZnTe, CdSe, and GaAs, and discuss the effects of shallow core states in comparison with other implementations such as the full potential linearized augmented planewave method. We will also compare our scheme with other Hartree-Fock pseudopotentials.

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