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Modeling of CeO2, Ce2O3, PrO2, and Pr2O3 in GGA+U formalism

안기용[1], 유동수[1], 이종호[2], 정용재[1]*

[1]한양대학교, [2]한국과학기술연구원

The electronic structure and various physical properties of CeO2, Ce2O3, PrO2, and Pr2O3 have been studied from the framework of Ab-initio by the all-electron projector-augmented-wave (PAW) method, as implemented VASP (Vienna Ab-initio Simulation Package). The generalized gradient approximation (GGA) with effective U (Ueff) has been used to explain the strong on-site Coulomb repulsion among the localized Ce 4f electrons. The dependence of selected observables of these materials on the Ueff parameter has been scrutinized. The studied properties contain lattice constants, density of states, and reaction energies of CeO2, Ce2O3, PrO2, and Pr2O3. For CeO2 and PrO2, the GGA(PBE)+U results are in good agreement with experimental data whereas for the computational calculationally more demanding Ce2O3 and Pr2O3 both approaches give comparable accuracy. This results represent that by choosing an appropriate Ueff it is possible to reliably describe structural and electronic properties of CeO2, Ce2O3, PrO2, and Pr2O3, which enables modeling of oxygen reduction reaction processes involving ceria-based materials.

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