Evidence of Coulomb correction and spinorbit coupling in rare-earth dioxides CeO_2, PrO_2 and TbO_2: An ab initio study

Abstract

The current study investigates the structural, elastic, electronic and optical properties of CeO_2, PrO_2 and TbO_2 using the full potential (linearized) augmented plane wave plus local orbital method within the WuCohen generalized gradient approximation (GGA) with Hubbard (U) **correction** and spinorbit coupling (SOC). The GGAU implementation lead us to describe correctly the relativistic effect on 4f electrons for CeO_2. We clarify that the inclusion of the Hubbard U parameter and the spinorbit coupling are responsible for the ferromagnetic insulating of PrO_2 and TbO_2. The magnetic description is achieved by the spin-density contours and magnetic moment calculations, where we show the polarization of oxygen atoms from the rare earth atoms. The mechanical stability is shown via the elastic constants calculations. The optical properties, namely the dielectric function and the reflectivity are calculated for radiation up to 12 eV, giving interesting optoelectronic properties to these dioxides