

Systematic study of the structural, electronic, optical and thermoelectric properties of $A\text{HfO}_3$ ($A = \text{Ca}, \text{Ba}$) perovskites at various pressure using ab-initio calculations

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ABSTRACT

The present study investigates the pressure dependence of the structural, elastic and electronic aspects for specifying the optical and thermoelectric device applications of alkaline rare-earth hafnate $A\text{HfO}_3$ ($A = \text{Ca}, \text{Ba}$) perovskites. The calculations have been performed by employing the all electron FP-LAPW+lo method. The PBEsol-GGA functional has been applied for treatment of the exchange-correlation energy. Using structural optimization, the lattice constants of the stable cubic phases are extracted, which are in good match with the existing theoretical and experimental literature. The cubic elastic constants (D_{11} , D_{12} and D_{44}), bulk moduli (B) are computed for evaluating the mechanical strength against external pressure up to 15 GPa. The electronic properties reveal that Hf-3d states primarily construct conduction band minima, while O-2p states construct valence band maxima at 0 GPa, exhibiting an indirect bandgap (Γ -M), which has been transformed to direct bandgap (Γ - Γ) at 15 GPa. Investigations of the optical properties illustrate that change in pressure can tune the optical parameters of these materials within ultra-violet (UV) energies suggesting commercial optoelectronic utilities. Our analysis shows that BaHfO_3 exhibits better thermoelectric properties than CaHfO_3 at room temperature whereas, thermoelectric performance both the compounds become comparable at higher temperature.

Key Words: $A\text{HfO}_3$ ($A = \text{Ca}, \text{Ba}$) perovskites; Under pressure study; Mechanical properties; Opto-electronic properties; Thermoelectric properties.