

The Contribution of Sr and Hf Atoms to the Piezoelectric Response of Tetragonal SrHfO₃

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Abstract

In this paper, the contribution of Sr and Hf atoms in piezoelectric properties of tetragonal SrHfO₃ with the P4mm space group were investigated, using first principle calculations based on density functional perturbation theory. Lattice constants, Born effective charges, piezoelectric constant, and the contribution of Sr and Hf to the total polarization and piezoelectric coefficient were calculated. Our results show that the tetragonal SrHfO₃ has a piezoelectric property, and its polarization and piezoelectricity mainly come from Hf atoms. The effect of lattice constant changes on the polarization and piezoelectric constant were also studied. It was found that the polarization and piezoelectric constant were enhanced by increasing the lattice parameter and at $c = 4.5 \text{ \AA}$, the Sr atom contributes to 50% of the total piezoelectric constant. This behavior is attributed to significant covalent bonding between Sr and the surrounding O atoms.

Keywords: piezoelectricity, Born effective charge, density functional perturbation theory, piezoelectric constant, lead-free piezoelectric

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