ELASTIC PROPERTIES AND BAND GAP TUNING OF CUBIC PEROVSKITE $SrHfO_3$: FIRST-PRINCIPLES CALCULATIONS FOR SOLAR ENERGY

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Abstract - Perovskite-type oxides due to their electrochemical properties, have received great interests for their applications in semiconducting devices like MOSFET. Among them $SrHfO_3$ with its 3.75 eV band gap and unique dielectric properties is of the most interesting perovskites. Density functional theory based first-principles calculations were used to study the mechanical and electronic properties of cubic $SrHfO_3$ using projector-augmented wave pseudopotential with PBEsol approximation. Investigating electronic properties shows that band gap variation trend is reduced to 2.4 eV in room temperature.

Keywords - Provskite, solar energy storing, Density Functional Theory; High order elastic constants; $SrHfO_3$.

I. INTRODUCTION

The ABO_3 perovskite type oxides have potentials to be attractive functional materials for their various unique properties. Among the perovskite compounds, $SrHfO_3$ has been proven to be one of the most promising high-κ dielectrics in MOSFET because of its great physical and electrical properties such as large band gap, optimal band offsets, high dielectric constant and high melting temperature and it has also been used in positron emission tomography, thermal barrier coating, etc. Using powder neutron diffraction, Kennedy and coworkers studied the high-temperature phase transitions of $SrHfO_3$ and observed three phase transitions as follows: Orthorhombic (Pnma, from 300 K to approximately 670 K) → orthorhombic (Cmcm, by 870 K) → tetragonal (I4/mcm, from ~1000 to 1353 K) → cubic (Pm3m, >1360 K). In view of $SrHfO_3$ as a highly promising dielectric gate in MOSFET application, it is of great importance and interest to study the elastic and electronic properties of cubic $SrHfO_3$.

The purpose of this work is to theoretically investigate the elastic constants, electronic band structure of cubic $SrHfO_3$. The paper is organized as follows: in section 2 describes the technical details and employed methods. Section 3 is devoted to the results and discussion of mechanical and electronic properties. We present our main conclusions in section 4.

II. COMPUTATIONAL METHODS

First principles study by DFT calculations were carried out using the projector-augmented wave (PAW) potentials which has been implemented in the QUANTUM ESPRESSO package [1] The correlation and exchange effects of the electrons were dealt with using the generalized gradient approximation (GGA) of Perdew-Burke-Ernzerhof (PBE) functional [2]. The kinetic energy cutoff for the plane wave basis set was chosen to be 600 eV. The Brillion zone was sampled with 8×8×8 k-points using the standard Monkhorst–Pack special grids [3]. Atomic positions were relaxed until the energy differences were converged within 10^{-6} eV and the maximum Hellmann– Feynman force on any atom was below 10^{-5} eV/Å. Electronic configurations which have been used for atoms Sr, Hf and O were [Kr] $5s^2$, [Xe] $4f^{14}5d^26s^2$ and [He] $2s^2$ $2p^4$, respectively.

III. RESULTS AND DISCUSSION

A. Atomic structure

Unit cell of $SrHfO_3$ can be seen in Fig. 1. In first step, lattice vector and atomic positions of the structure SrHfO3 have been optimized. Lattice vectors and bond lengths obtained using PBEsol approximation have been reported in Table 1 which is compared with similar compounds from other literatures.

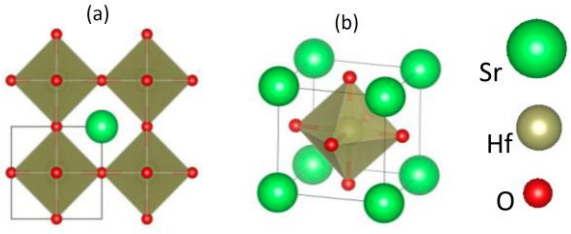


Fig. 1. Unit cell of $SrHfO_3$ from (a) top and (b) side views.

Method	a (Å)	Ref.
PBEsol	4.08	This work
Exp.	4.11	[12]

Table 1. lattice vectors and bond lengths of $SrHfO_3$.

B. Mechanical properties

To obtain energy-strain curves, the total energy of the structure was calculated under various deformation tensors. In every deformation tensor, by applying different amounts of mechanical loadings, a potential

well is realized. Here, the strain energy per atom is defined as: $E_s = (E_{tot} - E_0)/n$. where E_{tot} is total energy of the deformed $SrHfO_3$, E_0 is the total energy of the undeformed $SrHfO_3$ and n is the number of atoms in the unit cell. Figure 2 illustrates the Es -strain- curves for the $SrHfO_3$ exposed to three types of deformations.

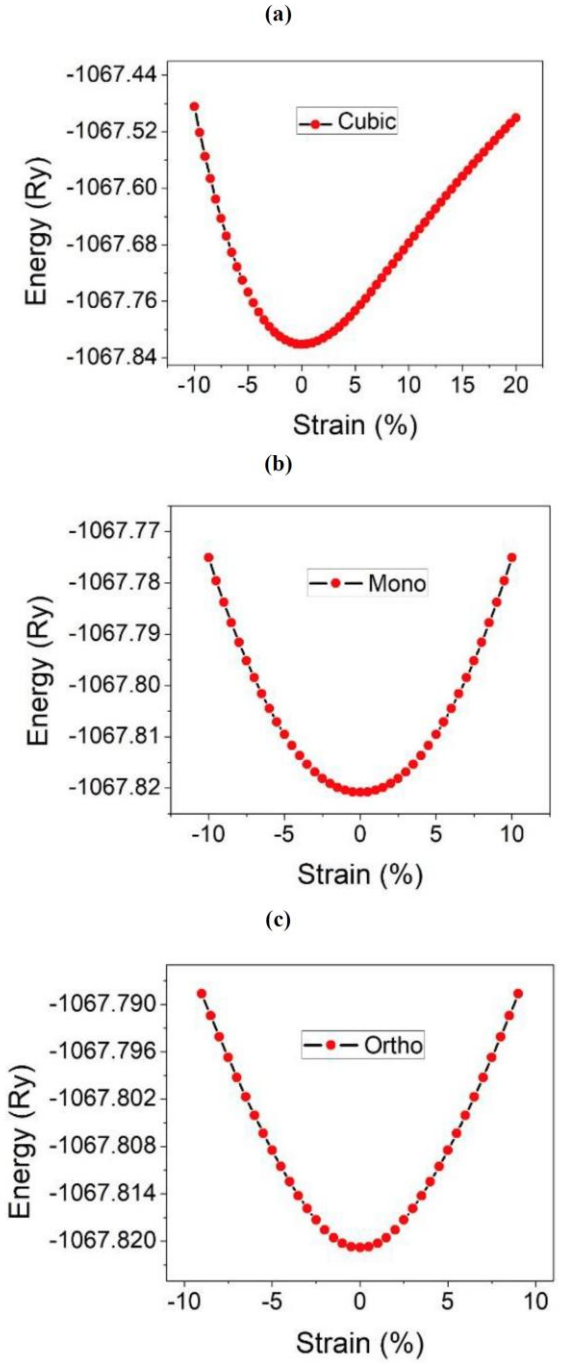


Fig. 2: Strain-energy curves for deformation (a) Cubic, (b) Ortho and (c) Mono.

C. Strain effects on the electronic properties of the CrN

Band structure of $SrHfO_3$ has been investigated, as seen in Figure 3. This material has indirect band gap of 3.75eV. Valence band maximum (VBM) of $SrHfO_3$ band structure is at point R in reciprocal space and conduction band minimum (CBM) is located at point Γ.

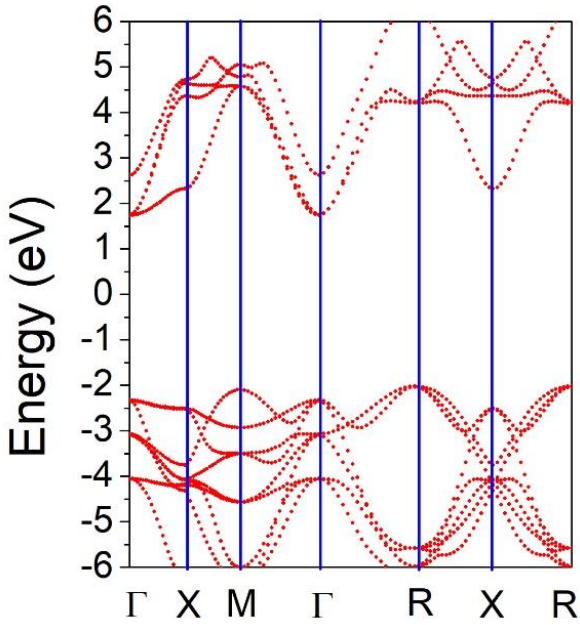


Fig. 4. Band structure of cubic SrHfO3.

Understanding from partial density of states (PDOS), shown in Figure 9, orbital 2P of O and 5D of Hf have the main role in formation of VBM and CBM, respectively.

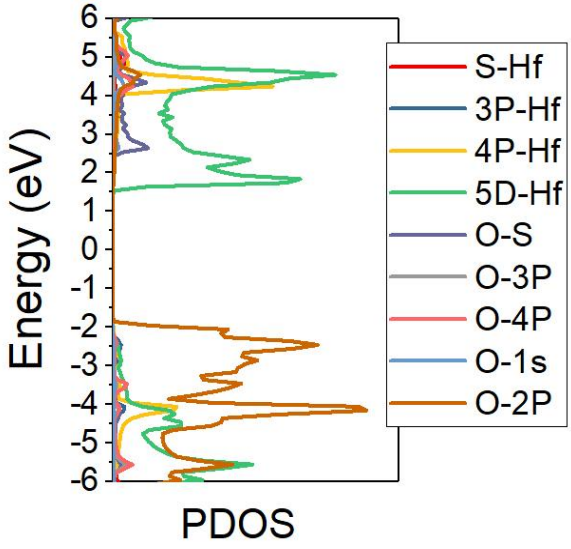


Fig. 5. PDOS of cubic SrHfO3.

IV. CONCLUSION

In this paper using exchange-correlation term revised for solids PBEsol alongside PAW pseudopotentials, we have made effort to compute elastic constants of cubic $SrHfO_3$ more aczcurate, utilizing revised calculation. Results show that our obtained values have greater agreement with experimental values in comparison other theoretical values reported in previous literatures.

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