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AN AB INITIO ANALYSIS OF STRUCTURAL, OPTICAL, ELECTRONIC, AND THERMAL PROPERTIES OF CUBIC $SrSnO_3$ USING WEIN2k[†]

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This paper investigated the structural, optical, electronic and thermal characteristics of $SrSnO_3$ perovskites that were calculated using the density functional theory. Software called WEIN2K is used to perform the calculation. According to our calculations, the band gap energy of the $SrSnO_3$ is roughly 4.00 eV and it adopts a distorted cubic shape in the space group $Pm\bar{3}m$. The band structure and partial density of state reflects the major contribution of O 2p in the valence band while 5s orbital from Sn in the conduction band. The electron density plot significantly shows the contribution different clusters SrO_{12} and SnO_6 that plays crucial role in electronic and optical properties. The creation of covalent bonds between the atoms of Sn and O as well as the ionic interaction between the atoms of Sr and O are both demonstrated by the electron density graphs and SCF calculation. The refractive index and extinction coefficient directly correlated with the real and imaginary part of complex dielectric function. Real part of dielectric function shows higher values at two major point of energy 3.54 eV and 9.78 eV associated with the absorption and optical activity of $SrSnO_3$. Negative part of imaginary dielectric function part suggests metallic behavior also supported by -grep lapw method. Thermoelectric and thermal conductivity properties suggest the power factor need to be improved for the device application.
Keywords: Density functional calculations; Electronic structure; Effective masses; Dielectric permittivity, Optical properties.
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The universal chemical formula for perovskite stannate oxides is $ASnO_3$ [1]. The alkaline earth stannate perovskites are one of the primary compounds in this group of minerals. Site A is occupied by alkaline earth metals including calcium (Ca), strontium (Sr), and barium (Ba), whose ionic radii vary from 100 pm to 135 pm [2]. In example, photovoltaic cells and light-emitting organic diodes have made extensive use of them to manufacture transparent electrodes for a variety of applications. Because of its outstanding dielectric and gas sensing qualities, $ASnO_3$ is very commonly utilised in electronics [3,4]. These perovskite compounds are used as anodes in Li-ion batteries and are made by destroying the crystal structure to produce sedentary metal oxides that are electrochemically active Sn metal. They are also promising materials for hydrogen synthesis and photocatalytic degradation [4,5].

The strontium stannate structure ($SrSnO_3$), which is the manuscript's main subject, is given special consideration. Sr^{2+} ions and 12 oxygen atoms occupy a dodecahedral site created by four [SnO_6] octahedrons to produce the crystalline structure of $SrSnO_3$ [6]. The Sn^{4+} cation is situated in the core of these octahedrons, which are made up of oxygen at their vertices. Due of the octahedral inclination that creates an orthorhombic structure (space group *Pbnm*) at ambient temperature, the unit cell of $SrSnO_3$ is a deformed cube [7]. Due to the extremely high mobility and concentration of carriers, SrSnO3 can also exist in other polymorphs (*Imma*, I4/mcm, and Pm3m) depending on the temperature increase [8].

In particular, $SrSnO_3$ is produced using a variety of synthesis techniques due to the scientific and technological interest in its applications. In order to clarify the effects of epitaxial tension on thin $SrSnO_3$ films, Gao et al. demonstrated that $SrSnO_3$ can be produced through a traditional solid-state reaction at high temperatures by combining an experimental investigation with a theoretical approach through DFT calculations using the LDA method [9]. Similar to this, a study conducted by Zhang et al. used DFT calculations implemented in the VASP simulation package, the revised Perdew-Burke-Ernzerhof function for solids (PBEsol) for structural relaxation, and Heyde-Scuseriae-Ernzerhof (HSE06) for the electronic structure analysis to explain the ferroelectricity induced by $SrSnO_3$ deformation and coupling, showing promising photovoltaic properties for use in solar cell devices [10].

Here, we carry out an ab-initio calculation for the strontium stannate structure ($SrSnO_3$) to show how the electrical properties are connected to various clusters, each of which has a distinct bonding environment based on the electron density distribution. Sr^{2+} ions are located in the corners of the cube in the crystal structure of $SrSnO_3$, while Sn ions are found with six oxygen atoms to form [SnO_6] octahedrons. The Sn^{4+} cation is situated in the core of these octahedrons, which are made up of oxygen at their vertices. $SrSnO_3$'s unit cell resembles a warped cube that produces an orthorhombic

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