



# Article A Comprehensive First-Principles Investigation of SnTiO<sub>3</sub> Perovskite for Optoelectronic and Thermoelectric Applications

Debidatta Behera <sup>1</sup>, Mumtaz Manzoor <sup>2</sup>, Ramesh Sharma <sup>3,\*</sup>, Mostafa M. Salah <sup>4,\*</sup>, Ivan Stich <sup>2</sup> and Sanat Kumar Mukherjee <sup>1</sup>

- <sup>1</sup> Department of Physics, Birla Institute of Technology, Mesra, Ranchi 835215, India
- <sup>2</sup> Institute of Informatics, Slovak Academy of Sciences, Dubravska cesta 9, 845 07 Bratislava, Slovakia
- <sup>3</sup> Department of Applied Science, Feroze Gandhi Institute of Engineering and Technology, Raebareli 835215, India
- <sup>4</sup> Electrical Engineering Department, Future University in Egypt, Cairo 11835, Egypt
- \* Correspondence: sharmadft@gmail.com (R.S.); mostafa.abdulkhalek@fue.edu.eg (M.M.S.)

**Abstract:** In this work, the structural, elastic, electronic, thermodynamic, optical, and thermoelectric properties of cubic phase SnTiO<sub>3</sub> employing first-principles calculation are examined. The calculations of all parameters via various potentials such as LDA, PBE-GGA, WC-GGA, PBEsol-GGA, mBJ-GGA, nmBJ-GGA, and HSE are performed. The computed band structure yields an indirect bandgap of 1.88 eV with the HSE approach. The optical parameters have been evaluated through absorption, dispersion, and loss function. For cubic phase SnTiO<sub>3</sub>, the maximum absorption coefficient  $\alpha(\omega)$  is  $173 \times 10^4 \text{ (cm)}^{-1}$  at high energy region 9 eV. The thermoelectric properties of the SnTiO<sub>3</sub> have been explored by the Seebeck coefficient, thermal conductivity, and power factor employing the BoltzTrap code with temperature and chemical potential. Furthermore, the thermodynamic quantities under high pressure (0–120 GPa) and temperature (0–1200 K) are also calculated.

**Keywords:** DFT; FP-LAPW; electronic properties; elastic properties; optical properties; thermoelectric properties; thermodynamic properties

# 1. Introduction

Over the last few decades, because of the rising need for energy around the world, the scientific community has become more interested in discovering new renewable energy sources. Owing to their excellent thermal efficiency, perovskite oxide compounds are useful in optoelectronic and thermoelectric usages such as thermoelectric coolers, thermocouples, etc. In the present scenario, perovskite ferroelectric materials are widely used in applications of electronics, IR sensors, non-volatile memories, dielectric properties, optical waveguides, and substrates for high- $T_{\rm C}$  superconductor growth [1,2]. Furthermore, perovskite compounds exhibit distinct properties such as low optical loss factor, high absorption in the invisible region, direct bandgap, etc. [1,3,4]. Due to these unique characteristics, semiconducting perovskites are promising candidates for usage in electronic devices that include solar cells, photodetectors, etc. [5–7]. To address the primary drawbacks of Pb-based perovskites, namely their toxicity and lack of chemical stability, numerous alternative perovskite compounds have recently been identified and synthesized. Gonjal et al. investigated Nb doped  $SrTiO_3$  and reported its thermoelectric properties [8]. According to these findings, lead-based perovskites can be effectively replaced with Snbased perovskites. SnTiO<sub>3</sub> is a potential Pb-free ferroelectric material with a high dielectric constant and ferroelectric polarization in theory. Nevertheless, most theoretical studies on SnTiO<sub>3</sub> materials focus only on their physical characteristics and strong polarization effects in the ferroelectric phase. The electrical and optical characteristics of the cubic structure of SnTiO<sub>3</sub> have undergone extensive theoretical and experimental studies [9-18]. The ferroelectric properties of the SnTiO<sub>3</sub> were reported by Parker et al. and others [19–21].



Citation: Behera, D.; Manzoor, M.; Sharma, R.; Salah, M.M.; Stich, I.; Mukherjee, S.K. A Comprehensive First-Principles Investigation of SnTiO<sub>3</sub> Perovskite for Optoelectronic and Thermoelectric Applications. *Crystals* 2023, *13*, 408. https:// doi.org/10.3390/cryst13030408

Academic Editors: Zhifang Shi and Guang Yang

Received: 28 January 2023 Revised: 14 February 2023 Accepted: 16 February 2023 Published: 27 February 2023



**Copyright:** © 2023 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (https:// creativecommons.org/licenses/by/ 4.0/). The primary structural motif in  $SnTiO_3$  is layers of honeycombs made of edge-sharing  $TiO_6$ -octahedra that are embellished with  $Sn^{2+}$  ions. The honeycomb lattice of edge-sharing  $TiO_6$ -octahedra along with the decoration of  $Sn^{2+}$  forms  $SnTiO_3$  [22]. Pielnhofer et al. forecast a significant tetragonal distortion of  $SnTiO_3$  as predicted by multiple GGA-based functionals [23]. In a cubic unit cell of  $SnTiO_3$ , Sn is at the corner of the cell whereas is O at the midpoint of each edge, and the Ti atom is in the center only. Due to the phase transition property of ferroelectric materials, SnTiO<sub>3</sub> exists in the cubic phase, having the space group Pm3m above 763 K, and transits to its paraelectric phase, while at ambient temperature it exhibits a tetragonal phase (P4mm) and transforms into ferroelectric material [24]. Mater et al. advocated the origin of the ferroelectric property of  $SnTiO_3$  in his study [25]. Konishi et al. [17] studied the electronic properties of the perovskite oxide  $SnTiO_3$  by using the plane-wave pseudopotential (PWPP) method. However, a bandgap of about 3-3.5 eV was reported in experiments, and the maximum value of 1.7 eV has been estimated from theoretical studies for SnTiO<sub>3</sub> in the paraelectric phase [9]. In an experiment, a group of researchers synthesized  $SnTiO_3$  thin film utilizing a deposition technique on  $LaAlO_3$  (001) substrate [26]. Due to its strong optical coefficient and photorefractive sensitivity,  $SnTiO_3$ is a potential candidate for optical sensors. Due to numerous mechanisms that allow the enabling of wide-bandgap photo voltages and increased efficiency, these materials are in high demand in emerging photovoltaic technologies. All such utilities of the material create an environment to investigate SnTiO3.

In the present work, thermoelectric properties along with optical properties of the cubic state of SnTiO<sub>3</sub> have been studied to use in optoelectronics and energy storage devices.

## 2. Computational Details

The full potential linearized augmented plane wave (FP-LAPW) method within the density functional theory (DFT) is used. This approach has been demonstrated to be one of the most precise approaches for computing the electrical structure of solids within DFT [27], as implemented in the WIEN2k code [28]. Using local density approximation (LDA), general gradient approximation with PBE-GGA, WC-GGA, and PBEsol GGA [29–32] exchange-correlation has been used to determine the optimized structure of the compound. On the other hand, new semi-local potentials known as TB-mBJ, nmBJ, and unmBJ [28,33] potentials were also used for electronic structure calculations to predict a more accurate bandgap compared to other potentials. The k-point sampling of the Brillouin zone is constructed using the Monkhorst Pack Mesh scheme with  $15 \times 15 \times 15$  grids in primitive cells of compounds with  $Rk_{max} = 7(R$ —the smallest muffin-tin radius and  $k_{max}$ —the cutoff wave vector of the plane-wave basis set) [34]. These parameters have been set for the convergence parameter for which the calculation stabilizes for the minimum energy [35]. The energy that separates the valence state from the core state has been chosen to be -6.0 Ry. The leakage electrons from the muffin-tin radius are found to be less than 0.0001e. The phonon spectrum of cubic SnTiO<sub>3</sub> was computed using the pseudo-potential plane-wave approach using VASP software [36]. The plane-wave cut-off was considered 450 eV for these computations. A denser k-mesh of  $18 \times 18 \times 18$  ( $\Gamma$ -cantered) is used for the IBZ integration of the unit cell. A supercell of  $3 \times 3 \times 3$  consisting of 135 atoms and k-mesh  $9 \times 9 \times 9$  for the phonon frequencies is employed.

#### 3. Results and Discussion

#### 3.1. Structural Properties

The crystal structure of cubic SnTiO<sub>3</sub> is represented in Figure 1. The total energy variation with a volume of SnTiO<sub>3</sub> considering different potentials such as LDA, PBE-GGA, WC-GGA, and PBEsol-GGA is shown in Figure 2a–d, which determines that the equilibrium lattice constant a = 3.9511 Å is in good agreement with earlier theoretical findings [13,37,38]. The optimized lattice parameter is observed to be slightly higher than the experimental findings. Murnaghan's equation of states is considered for conducting structural relaxation [39] for volume optimization. From the optimized fit curve, the basic

structural parameters are measured. The calculations show that the best fitting is observed using potential PBE-GGA, where the maximum energy is obtained, which shows material  $SnTiO_3$  is the more stable, as represented in Table 1. The computed lattice parameters are observed and follow the earlier studies [40].



Figure 1. Crystal structure of cubic SnTiO<sub>3</sub>.

**Table 1.** Estimated lattice parameter *a* (Å), bulk modulus *B*, bulk modulus derivative *B*<sub>*P*</sub>, the minimum total energy *E*<sub>tot</sub>, the energy of cohesion *E*<sub>coh</sub>, enthalpy of formation *E*<sub>*f*</sub>, and bond length (Å).

Parameters		SnTiO <sub>3</sub> (Cubic)	
LDA	This study	Others' Theory	Exp.
$a(\text{\AA})$	3.8731	3.850 [41]	3.960 [42]
$V(\text{\AA})^3$	392.0831		
B(GPa)	209.2639		
$B_P$	4.6452		
$E_0(\mathrm{Ry})$	-14,500.9203		
PBE-GGA			
<i>a</i> (Å)	3.9511		
$V(\text{\AA})^3$	416.2415		
B(GPa)	175.1369		
B.P	4.5807		
$E_0(\mathrm{Ry})$	-14,517.819155		
WC-GGA			
a(Å)	3.9069	3.910 [43]	
$V(\text{\AA})^3$	402.4362		
B(GPa)	194.3111		
$B_P$	4.5816		
$E_0(\mathrm{Ry})$	$-14,\!514.870912$		
PBEsol-GGA			
a(Å)	3.9078	Ref. 3.916 [44]	
$V(\text{\AA})^3$	402.7150		
B(GPa)	191.0451		
$B_P$	4.2555		
$E_0(\mathrm{Ry})$	-14,508.909256		
Formation	-2 578		
energy(eV/atom)	2.070		
$E_{coh}(eV)$	-17.600	-37.088 [45]	
٥	Sn-Sn = 4.07		
Bond length (Å)	Sn-O = 2.818		
	Ti-O = 2.0378		



**Figure 2.** Variation in total energy with volume for cubic SnTiO<sub>3</sub> obtained using (**a**) LDA, (**b**) PBE-GGA, (**c**) WC-GGA, (**d**) PBEsol-GGA, and (**e**) the combined phonon dispersion and TDOS of SnTiO<sub>3</sub> compound.

Other physical characteristics, such as bulk modulus and the pressure derivatives of the bulk modulus, are estimated using potential PBE-GGA represented in Table 1. The device's design considers compound stability. As a result, we have identified the structural and mechanical stabilities of  $SnTiO_3$  employing the Born mechanical stability condition Goldschmidt tolerance factor, etc. The tolerance factor ( $t_G$ ), which is derived from the relation, demonstrates the magnitude of the strain forces acting on the structure.

$$t_G = \frac{r_{Sn} + r_O}{r_{Ti} + r_O} \tag{1}$$

where  $r_{Sn}$ ,  $r_{Ti}$  and  $r_O$  are the radii of Sn, Ti, and O atoms. A tolerance factor in the range of 0.93 to 1.04 is ideally suited for stable compounds; any variation on it induces additional force to the structure that significantly affects the material properties. The estimated values

of the SnTiO<sub>3</sub> tolerance factor are within the permitted range, indicating that SnTiO<sub>3</sub> is structurally stable. Additionally, the following relationship is used to extrapolate the thermodynamic stability from the enthalpy of the formation.

$$\Delta H_f = E_{bulk}^{SnTiO_3} - E_{bulk}^{Sn} - E_{bulk}^{Ti} - 3E_{bulk}^O$$
<sup>(2)</sup>

Here,  $E_{bulk}^{Sn}$ ,  $E_{bulk}^{Ti}$ , and  $E_{bulk}^{O}$  are bulk energies of the investigated compound and  $E_{bulk}^{SnTiO_3}$  is the total energy in bulk form. The calculated enthalpy of formation is -2.578 eV/atom, suggesting the stability of SnTiO<sub>3</sub>.

To confirm the stability of the SnTiO<sub>3</sub> compound, the phonon dispersion (PD) against momentum is computed and illustrated in Figure 2e. In a scattering association plot, the modes typically resemble spaghetti. A phonon dispersion correlation with distinct transverse and longitudinal modes [46]. We took the frequency (THz) along the y-axis with a range from (0 THz to 25 THz) and momentum along the x-axis. Almost all modes lie in the positive frequency having the real phonon branches, suggesting the stability of the investigated SnTiO<sub>3</sub> [47,48].

## 3.2. *Elastic Properties*

Elastic properties are the key parameter in determining the mechanical profile of the compound, such as bulk modulus (*B*), brittleness, stiffness, ductility, and isotopic character. The ratio of change in pressure to volume compression is known as bulk modulus (*B*) and is expressed as

$$B = -V\frac{\partial P}{\partial V} \tag{3}$$

The elastic constants are calculated by using the derivatives of energy as a function of lattice strain Calculation of Elastic Constants using the Method of Crystal Static Deformation [34]:

$$C_{ijkl} = \left(\frac{\partial\sigma_{ij}}{\partial\varepsilon_{jkl}}\right)_0 = \left(\frac{1}{V}\frac{\partial^2 E}{\partial\varepsilon_{ij}\partial\varepsilon_{kl}}\right)_0 \tag{4}$$

To compute elastic constants, the program IRELAST is used [49]. In the case of a cubic compound, three independent stiffness constants  $C_{11}$ ,  $C_{12}$ , and  $C_{44}$  are determined by retaining suitable lattice distortions. These constants,  $C_{11}$  and  $C_{12}$ , can be computed from the stress–strain relation by applying  $\varepsilon_1$  strain. These are defined as:

$$C_{11} = \frac{\sigma_1}{\varepsilon_1} \text{ and } C_{12} = \frac{\sigma_2}{\varepsilon_1}$$
(5)

for 
$$\sigma_4$$
,  $\sigma_4 = C_{44}\varepsilon_4$  (6)

The calculation shows positive values of elastic constant and satisfies the mechanical stability criteria [50].

$$C_{11} - C_{12} > 0, (7)$$

$$C_{11>0}$$
, (8)

$$C_{44} > 0,$$
 (9)

$$C_{11} + 2C_{12} > 0 \tag{10}$$

The bulk modulus also satisfies the criteria:  $C_{12} < B < C_{11}$ 

The elastic compliance tensor, which is well-connected in relation with the elastic components, is as follows:

$$S_{11} = \frac{(C_{11} + C_{12})}{[(C_{11} - C_{12})(C_{11} + 2C_{12})]}$$
(11)

$$S_{12} = \frac{(-C_{12})}{[(C_{11} - C_{12})(C_{11} + 2C_{12})]}$$
(12)

$$S_{44} = \frac{1}{C_{44}} \tag{13}$$

Following is the relationship between elastic constants, bulk modulus *B*, and the compressibility  $\beta$ :

$$B = \frac{1}{\beta} = \frac{C_{11} + 2C_{12}}{3} \tag{14}$$

In a cubic compound, the shear modulus *G* and the isotropy factor *A* are each specified as [51]:

$$G = \frac{C_{11} - C_{12}}{2}$$
 and  $A = \frac{C_{11} - C_{12}}{2C_{44}}$  (15)

The estimated elastic constants are under the Born mechanical condition for stability requirements  $C_{11} - C_{12} > 0$ ,  $C_{11} + 2C_{12} > 0$ ,  $C_{44} > 0$ , and  $C_{12} < B < C_{11}$ , which suggests the investigated compound is mechanically stable. The  $C_{11}$  is higher and stiffer than  $C_{12}$  and  $C_{44}$ , while  $C_{44}$  is higher than  $C_{12}$ . As a result, the stabilities highlight the significance of  $SnTiO_3$  in device manufacture. The computed values of Shear modulus (G), Bulk modulus (B), etc., are presented in Table 2. To ascertain a material's ductile or brittle nature, Pugh's Ratio (B/G) and Poisson ratio ( $\upsilon$ ) are considered, and limits for brittle nature are B/G < 1.75 and v < 0.26 [49]. The studied SnTiO<sub>3</sub> is brittle by nature as evidenced by the above parameters, represented in Table 2. Furthermore, Cauchy pressure  $C_{12}$ - $C_{44}$  supports this. The positive magnitude of C<sub>12</sub>-C<sub>44</sub> reveals the compound is ductile, whereas the negative magnitude suggests brittle. The Poisson ratio v is around 0.25, indicating that most of the bonding in the materials is ionic [52]. The isotropic/anisotropic nature of the investigated  $SnTiO_3$  can be ascertained from the anisotropic factor (A). Having A = 1 suggests an isotropic nature, whereas anything other than 1 reflects an anisotropic character [53]. The investigated compound is found to be elastically anisotropic, as obtained from Table 2. The melting temperature was observed to have an increased nature for  $SnTiO_3$ , as indicated in Table 2.

**Table 2.** Calculated elastic constants  $C_{11}$ ,  $C_{12}$ ,  $C_{44}$  (in GPa); Bulk modulus B (in GPa); shear modulus G (in GPa); Young's modulus E (in GPa); Poisson's ratio ( $\sigma$ ); B/G ratio; Cauchy pressure; Zener anisotropy factor (A); Debye temperature ( $\Theta_D$ ) in K; transverse velocity ( $v_t$ ); longitudinal velocity ( $v_1$ ); and average velocity ( $v_{avg}$ ) in m/s and melting temperature Tm (K) for SnTiO<sub>3</sub>.

Material Property	SnTiO <sub>3</sub>	<b>Ref.</b> [44]	<b>Ref.</b> [43]
C <sub>11</sub> (GPa)	220.36	314.69	356.79
C <sub>12</sub> (GPa)	97.96	119.62	132.93
C <sub>44</sub> (GPa)	100.2846	94.06	90.47
Bulk modulus, B (GPa)	138.764	184.64	207.55
Shear modulus, G (GPa)	82.265		
Young's modulus, Y (GPa)	206.072		
Poisson ratio, σ (GPa)	0.252		
Pugh ratio, B/G (GPa)	1.68		
Frantsevich ratio, G/B (GPa)	0.59		
Shear anisotropy factor, A (GPa)	1.63		
Cauchy pressure C <sup>P</sup> (GPa)	-2.32		
Transverse sound velocity (m/s)	3772.96		
Longitudinal sound velocity (m/s)	6556.84		
Average sound velocity (m/s)	4189.92		
Debye Temperature $\Theta_{D}$ (K)	539.942		
Melting temperature T <sub>m</sub> (K)	$1855.3660 \pm 300 \ {\rm K}$		

#### 3.3. Electronic Structure

The energy band structure and total and partial density of states (TDOS and PDOS) determine the electronic properties of  $SnTiO_3$ . Along high symmetry axes, the electronic band structure of SnTiO<sub>3</sub> is plotted using potentials LDA, PBE-GGA, WC-GGA, PBEsol-GGA, mBJ, nmBJ, un-mBJ, and HSE approximation, as shown in Figure 3a-h. The estimated bandgap is 1.002 eV, 1.373 eV, 1.080 eV, 1.065 eV, 1.415 eV, 1.451 eV, 1.347 eV, and 1.881 eV using LDA, PBE-GGA, WC-GGA, PBEsol-GGA, mBJ-GGA, nmBJ-GGA, unmBJ-GGA, and HSE approaches, respectively. From the density of states plotted in Figure 4a, the splitting of various states can be noticed that were affected by the electrostatic interaction of O-2p orbitals. The uppermost level of the valence band is considered zero from the fermi level. Furthermore, it is observed that the topmost of the valence band at point *X* and the bottom of the conduction band at  $\Gamma$  refer to an indirect bandgap for the studied compound. O-2p and Ti-3d orbitals belong to the valence band and conduction band, respectively, whereas Sn and O exhibit a strong covalent bonding. This covalent bonding confirms the excellent behavior of ferroelectric material in the SnTiO<sub>3</sub> compound [45]. Comparative calculated bandgaps in this work and other reported theoretical and experimental works for  $SnTiO_3$  are represented in Table 3. It asserts that our findings are consistent with prior experimental and theoretical findings [54,55]. The computed band gap values advocated that this material is suitable for optoelectronic devices because each potential bandgap value is within the visible region.

**Table 3.** Comparison between Calculated Bandgaps and Reported Theoretical and Experimental Bandgaps for SnTiO<sub>3</sub>.

	Banc	lgaps
	Sn	ГіО <sub>3</sub>
XC	Present Work	Others' Works
LDA	1.002	
PBE-GGA	1.373	1.164 eV [45]
WC-GGA	1.080	
PBEsol-GGA	1.065	2.445 eV [44]
mBJ-GGA	1.415	
nmBJ-GGA	1.451	
unmBJ-GGA	1.347	
HSE	1.88	



**Figure 3.** SnTiO<sub>3</sub> of band structures at their equilibrium lattice constants estimated using (**a**) LDA, (**b**) PBE-GGA, (**c**) WC-GGA, (**d**) PBEsol-GGA, (**e**) mBJ, (**f**) nmBJ, (**g**) unmBJ, and (**h**) HSE approximation.



**Figure 4.** (a) Total DOSs for SnTiO<sub>3</sub> obtained using the LDA, PBE-GGA, WC-GGA, PBEsol-GGA, mBJ, nmBJ, unmBJ, and HSE06. (b) Partial density of states (PDOS) for SnTiO<sub>3</sub> obtained using the nmBJ-GGA potential.

The density of states (DOS) advocates the number of states that can be occupied per period of energy at each energy level [56]. Figure 4a,b represents the partial density of states (PDOS) as well as the total density of states (TDOS) for investigated SnTiO<sub>3</sub>. The upper valence band is dominated by O-2p electrons for all compositions of compounds, and the lower valence band originates from Ti-3d, Sn-5p. With a wider extension for SnTiO<sub>3</sub>, the empty Ti(3d) is centered above  $E_V$  within the conduction band (CB) at 4 eV. The bandgaps obtained from the band structure exactly match the bandgap obtained from the density of the state's plot. From Figure 4a, it is observed that when using the LDA, PBE-GGA, WC-GGA, PBEsol-GGA, mBJ-GGA, nmBJ-GGA, unmBJ-GGA, and HSE approaches, the calculated bandgap is 1.002 eV, 1.373 eV, 1.080 eV, 1.065 eV, 1.415 eV, 1.451 eV, 1.347 eV, and 1.881 eV, respectively, for SnTiO<sub>3</sub> perovskite.

To analyze the charge transfer phenomenon and bonding characteristics, the charge density is computed in (100) and (110) planes, as represented in Figure 5a,b. It reveals the presence of significant hybridization between Ti-3d and O-2p orbitals [57]. The Bader charge analysis confirms the ionic character of O that accepts the electrons from Sn and Ti. The numerical values of Bader charge for Sn, Ti, and O are +1.41, +2.07, and -1.16, respectively, which support the strong hybridization.



(a)

(b)

**Figure 5.** Valence electron charge density contour plot of SnTiO<sub>3</sub> using GGA-mBJ (**a**) (100) plane in 3D representation and (**b**) (110) plane charge density contour plot SnTiO<sub>3</sub>.

# 3.4. Optical Properties

The compound SnTiO<sub>3</sub> material is one of the future-efficient materials for solar cells due to its band gap. This has a high optical response to the electromagnetic spectrum. To analyze the optical behavior of the material, the SnTiO<sub>3</sub> compound was studied by applying the electromagnetic on the surface of the material. The analysis of frequency-dependent linear optical properties, namely, the imaginary part of the dielectric function  $I\varepsilon_{\alpha\beta}(\omega)$ , real part of the dielectric function  $R\varepsilon_{\alpha\beta}(\omega)$ , electron energy function  $L(\omega)$ , reflectivity  $R(\omega)$ , and absorption coefficient  $\alpha(\omega)$  of cubic SnTiO<sub>3</sub> were performed using the nmBJ-GGA method. The results in Figure 6a–d show the numerical analysis, which is presented in Table 4.

The predicted optical properties of cubic SnTiO<sub>3</sub> in the range 0–10 eV are represented in Figure 6a–d. The physical explanation of the peaks observed in the optical spectra is the transition of electrons from occupied to unoccupied energy levels along high symmetry points in the Brillouin zone [4]. The real  $\varepsilon_1(\omega)$  and imaginary parts  $\varepsilon_2(\omega)$  of the dielectric function for SnTiO<sub>3</sub>, as shown in Figure 6a,b, are computed using the following relationship.

$$\varepsilon_1(\omega) = 1 + \frac{2}{\pi} P \int_0^\infty \frac{\omega' \varepsilon_2(\omega')}{\omega'^2 - \omega^2} d\omega'$$
(16)

$$\varepsilon_2(w) = \frac{4\pi e^2}{m^2 \omega^2} \sum_{ij} \int \langle i|M|j \rangle I^2 f_i (1 - f_i) \delta\Big(E_f - E_i - \omega\Big) d^3k \tag{17}$$

In the dielectric constant  $\varepsilon_1(\omega)$  and  $\varepsilon_2(\omega)$  analysis, the transition of electronics or dispersion and absorption of electrons at the zero-frequency, as well as the visible region, are examined. Additionally, Table 4 provides the computed value of  $\varepsilon_1(\omega)$  at 0 eV, which is termed a static dielectric constant  $\varepsilon_1(0)$ . The transition steadily grew after  $\varepsilon_1(0)$  with a maximum value of about 2.90 eV, as shown in Figure 6a. The peaks continuously fall as photon energy rises, reaching a negative value at 6.15 eV. The negative dielectric suggests the metallic nature of the SnTiO<sub>3</sub> after 6.15 eV. The computed outcomes are under Penn's model via the relationship  $\varepsilon_1(0) \approx 1 + D (E_p/E_g)$ , where *D* stands for constant factor whose value is about unity,  $E_p$  is the plasma energy, and  $E_g$  is the average gap in the first Brillouin zone [59]. The estimated results are consistent with the model referring to the reliability of the compound. Figure 6a also presents the imaginary part  $\varepsilon_2(\omega)$  in the 0–10 eV energy range. At the static point, there is no absorption while increasing the energy (eV). Because of absorptive transitions from the Valence band (VB) to the Conduction Band (CB), these peaks appeared. When the value of photon energy (eV) crossed the band gap, values then started the gradual absorption and gave the maximum value of absorption of almost 12.6 at 5.1 eV.



**Figure 6.** Spectra of the (**a**) real  $\varepsilon_1(\omega)$  and imaginary  $\varepsilon_2(\omega)$  dielectric functions, (**b**) refractive indices  $n(\omega)$  and extinction coefficient  $K(\omega)$ , (**c**) Absorption coefficient  $\alpha(\omega)$ , and (**d**) conductivity against photon energy (eV) of cubic SnTiO<sub>3</sub> obtained using the nmBJ-GGA method.

Demonster	SnT	ſiO <sub>3</sub>
Parameter	Present Work	Others' Works
$\varepsilon_1(0)$	6.51	7.15 [4]
<i>n</i> (0)	2.54	2.67 [4]
R(0)%	0.18	0.21 [58]

Table 4. Calculated and Reported Theoretical optical properties for SnTiO<sub>3</sub>.

Figure 6b presented the combined refractive index  $n(\omega)$  as well as the extinction coefficient  $k(\omega)$ . The refractive index  $n(\omega)$  provides information regarding the transparency of investigated compounds when photons of the light incident and the extinction coefficient  $k(\omega)$  examined the resistance of electrons on their surface [60]. The magnitude  $n(\omega)$  gets close to zero when the compound is completely transparent. The estimated values of  $n(\omega)$  are mentioned in Table 4. The maximum value  $n(\omega)$  lies at 2 to 3 as visible light is examined, as shown in Figure 6b. It attains a peak value at 2.54 eV that belongs to resonance frequency, which is observed to be identical to the  $\varepsilon_1(\omega)$  trend, and then starts decreasing. Depending on the wavelength, a difference in the refractive index separates light into its colors [61]. As a result, the trajectory of the  $n(\omega)$  plot is comparable to  $\varepsilon_1(\omega)$  as per  $n^2 - k^2 = \varepsilon_1(\omega)$ , as represented in Figure 6b. Additionally, the static refractive index belongs to the zero energy level as n(0) and the real dielectric constant are strongly correlated,  $n^2(0) = \varepsilon_1(0)$ , as

represented in Table 4. As seen in Figure 6b, the plot of extinction coefficient  $k(\omega)$  is just the replica of  $\varepsilon_2(\omega)$ . Additionally, it demonstrates that in the ultraviolet portion, light is mostly absorbed. Like the absorption, the extinction coefficient  $k(\omega)$  shows no resistance to the static value. On the other hand, by increasing the photon energy (eV), the resistance starts and is found to have the highest resistance of 2.1 at 2.9 eV. After that, it decreases by increasing the energy (eV). Figure 6c demonstrated the optical conductivity ( $\sigma$ ) of the material by falling the photon light on the material. The amount of free carriers generated is quantified by optical conductivity  $\sigma(\omega)$ , which is an outcome of bond disruption caused by photon–electron interaction [62]. At the static point, there is no conductivity, and similar behavior to absorption by enhancing the photon energy (eV) increases the conductivity. We examined the maximum conductivity from 4.5 eV to 5 eV for the SnTiO<sub>3</sub> compound, as illustrated in Figure 6c. As shown in Figure 6d, it is evident that light starts absorbing at 1.46 eV. This is obvious as the energy of incoming light is consistent with the bandgap of the investigated compound. Maximum light absorption is recorded in the ultraviolent region, as evidenced by the peak at 9.97 eV. At this region, maximum absorption is found to be  $(173 \times 10^4$ /cm), suggesting the materials investigated are ideally suited for optoelectronic applications. The entire study shows that the examined material is a suitable candidate for optoelectronic applications due to maximum absorption, low optical loss, and the presence of bandgap in the visible region.

#### 3.5. Thermodynamic Properties

To analyze the material nature in the dynamics form, the thermodynamic properties are computed. In Figure 7a, the specific heat  $C_V$  is plotted against temperature at various values of pressure. It is observed from Figure 7a that with increasing pressure, specific heat  $C_V$  decreases at the same value of temperature. The value of specific heat  $C_V$  increases when temperature increases at the same value of pressure. The specific heat  $C_V$  increases rapidly with the rising of the temperature up to T < 500 K because the volume of the investigated compound changes more in this range. The specific heat  $C_V$  is near to the Dulong–Petit limit at T > 900 K [63].



**Figure 7.** (a) Specific heat, (b) Grüneisen parameter, (c) thermal expansion coefficient, (d) bulk modulus, (e) Debye temperature, (f) Entropy vs. Temperature of cubic SnTiO<sub>3</sub> obtained using the nmBJ-GGA method.

The thermodynamic Grüneisen parameter ( $\gamma$ ) holds importance when used to quantify the relationship between thermal and elastic properties [61], as shown in Figure 7b. It

is plotted against temperature at a series of pressures for SnTiO<sub>3</sub> in Figure 7e. At 0 GPa pressure, the Grüneisen parameter  $\gamma$  increases up to 2.250 gradually at different values of temperature; however, at high pressures, no significant change is observed in the Grüneisen parameter ( $\gamma$ ).

The structural stability of the compound is explicated by the thermal expansion coefficient  $\alpha$ . Figure 7c shows the temperature influence on the thermal expansion coefficient. It is evident that, initially, when temperature T rises from 0 K to 300 K, the thermal expansion coefficient increases significantly at 0 GP of pressure. Its value becomes  $3.8 \times 10^5$ /K at 300 K at a certain value of 0 GPa pressure. More likely, it is somehow sensitive at 0 GPa pressure. Additionally, at a specific temperature, thermal expansion reduces as pressure rises. This demonstrates that under high pressure, SnTiO<sub>3</sub> exhibits significant volume variance. Thus, we can say that increasing the value of temperature and pressure both indicate opposite effects on the thermal expansion coefficient  $\alpha$ .

The bulk modulus of SnTiO<sub>3</sub> at different values of pressure and temperature is investigated, and results are shown in Figure 7d. The value of bulk modulus remains unchanged in the temperature range of 0 K < T K < 100 K at all pressure values. After this temperature range, the *B* value drastically decreases linearly in the temperature range of 100 K < T < 1000 K. By maintaining the temperature constant, it can be noticed that the bulk modulus rises with rising pressures. Inversely, the compressibility, which is an inverse of bulk modulus, increases with increasing temperature at a certain temperature. Additionally, compressibility decreases with increasing pressure at the same temperature. In any crystal lattice, Debye temperature [59,64] not only imitates the degree of dynamic distortion but is a crucial point of the bonding between the atoms and substances. In Figure 7e, Debye temperature gives a maximum value of 1100 K at a high pressure of 120 GPa. The entropy of SnTiO<sub>3</sub> increases with an increase in the temperature from 0–1200 K and is observed to decrease with an increase in pressure.

#### 3.6. Thermoelectric Properties

Thermoelectric materials can transfer thermal energy directly to electrical energy [65,66]. Perovskite materials with improved thermal efficiency and a high absorption coefficient are important for thermoelectric applications due to their capacity to transform thermal energy into electrical energy [65–67], which makes them potential candidates for thermoelectric applications [68–72]. The thermoelectric properties of the compounds are computed using the Boltzmann transport theory as employed in the BoltzTrap program with a dense k mesh  $46 \times 46 \times 46$ , which is the converged value. The thermoelectric figure of merit *ZT* [66,73], which is the conversion efficiency of thermoelectric devices, is quite low, defined below as,

$$ZT = S^2 \frac{\sigma T}{\kappa}$$

where *S* represents the Seebeck coefficient,  $\sigma$  is the electronic conductivity, *T* is the absolute temperature, and  $\kappa$  is the thermal conductivity. Thermal conductivity ( $\kappa$ ) is divided into lattice thermal conductivity  $\kappa_l$  and electronic thermal conductivity  $\kappa_e$ . For the best *ZT*,  $\sigma$  and *S* should be high but  $\kappa$  should be low [74]. Figure 8a–d plots the thermoelectric properties with temperature.

The electrical conductivity ( $\sigma$ ) increases with the temperature and attains maximum values  $11.65 \times 10^{18} (\Omega \cdot m \cdot s)^{-1}$  at 1200 K, as mentioned in Figure 8. Electrical conductivity increases because of the narrower band gap, which forces the carriers to exert more energy to migrate toward the conduction band. Figure 8d shows the variation of electrical conductivity with chemical potential at different temperatures (300, 600, 900, 1200 K). From the plot, we analyze that the compound delivers high  $\sigma$  to achieve high efficiency for the thermoelectric system [75]. The electrical conductivity observed a rising pattern with chemical potential, as shown in Figure 8d. For p-type doping, the greatest electrical conductivity is perceived. The numerical magnitude of electrical conductivity at room temperature at 300 K is represented in Table 5.



**Figure 8.** (a) Electrical conductivity, (b) thermal conductivity, (c) Seeback coefficient vs. temperature, (d) electrical conductivity, (e) thermal conductivity, and (f) Seeback coefficient vs. the chemical potential of cubic obtained using the nmBJ-GGA method.

Table 5. Calculated thermoelectric properties at 300K for SnTiO<sub>3</sub>.

<b>D</b> (	Sn	TiO <sub>3</sub>
Parameter —	Present Work	Others' Works [76]
$\Sigma (\Omega ms)^1 (10^{18})$	1.50	2.5
K <sub>tot</sub> (W/mKs) (10 <sup>15</sup> )	0.76	1.8
$S(\mu V/K)$	247	90
$\frac{P.F}{(W/K^2ms10^{10})}$	1.50	2

Generally, thermal conductivity ( $\kappa$ ) originated due to electrons and lattice vibration. Both the electronic and the phonon contributions have been examined in this study. Figure 8b shows the variation of estimated total thermal conductivity for SnTiO<sub>3</sub>. Its value decreases with temperature and attains a minimum magnitude of  $0.23 \times 10^{15}$  (W/mKs) due to improved carrier concentration. Wiedemann Franz's law ( $=\frac{\kappa}{\sigma}$ ) [61] establishes the relative relationship between thermal and electrical conductivity [77]. The ratio of  $\frac{\kappa}{\sigma}$  is in the order of  $10^{-5}$ , which refers to high electrical conductivity but low thermal conductivity.

Another key factor associated with electronic band structure is known as the Seebeck coefficient, which is closely related to band structure and reveals the nature of dominant charge carriers. The chemical potential and temperature dependencies are also important factors for understanding the doping contribution of the perovskites S determines the variety of leading transporters. The negative value of S displays n-type but the positive value of S denotes p-type materials. Thus, p and n types of doping are equally effective in achieving a high value of S. This is plotted against temperature and chemical potential, as shown in Figure 8c,f, at different temperature ranges. The oscillation, with peaks at both positive and negative values, illustrates the potential variation. The peaks show a higher intensity for positive potential than peaks of low intensity with negative potentials due to a smaller number of electrons than the number of holes, which means a suitably large

S value can be performed by lesser *p* or *n* doping types. A comparison of thermoelectric properties at room temperature (300 K) is studied and mentioned in Table 5.

The thermoelectric efficiency of the investigated compound is addressed by considering the power factor (PF) and figure of merit (*ZT*) [78]. S needs to be high to reach a maximum power factor. At different temperatures (300–1200 K), as a function of chemical potential between -2 eV and 2.0 eV, the influence of chemical potential on the power factor has been examined, as shown in Figure 9c. The ideal power factor, or PF, has a value for p-type carriers of  $6.67 \times 10^{11} \text{ W/K}^2\text{ms}$ , which informs us about the performance of thermoelectric materials. The figure of merit has been used to compute the thermoelectric efficiency (*ZT*). As shown in Figure 9b, the value of the figure of merit grows from 0 to 0.34 between 100 K and 1200 K, which is highly significant for the best thermoelectric materials. According to the results of the current study, SnTiO<sub>3</sub> is therefore suitable for thermoelectric applications such as thermoelectric generators.



**Figure 9.** (a) Power factor, (b) *ZT* vs. temperature, (c) power factor, and (d) *ZT* chemical potential of cubic obtained using the nmBJ-GGA method.

#### 4. Conclusions

Using the FP-LAPW approach and the framework of density functional theory, we have comprehensively examined the structural, elastic, electronic, thermodynamic, and thermoelectric properties of cubic perovskite SnTiO<sub>3</sub> in this study (DFT). In this study, we have calculated the bulk modulus, Pugh ratio, and anisotropy factor of compound SnTiO<sub>3</sub>. The compound under consideration is brittle, and all elastic properties are intimately related to the crystal structure and the type of bonding between the atoms. We observed that the Grüneisen parameter  $\gamma$  increases up to 2.250 gradually at different values of temperature for SnTiO<sub>3</sub>. The Debye temperature shows a maximum value of 1100 K at a high pressure of 120 GPa, and the specific heat  $C_V$  is close to the Dulong–Petit limit at T > 900 K. We compared the results obtained by using HSE potential with those calculated by using various potentials such as LDA, PBE-GGA, WC-GGA, PBEsol-GGA, and nmBJ-GGA. The electronic properties have calculated a maximum indirect bandgap of 1.881 eV for nmBJ-GGA as compared to the other approximations and the Sn-5d and O-2s states predominate below the Fermi level according to the assessment of the overall density of states. Additionally, we computed the optical properties for maximum transition and

absorption found against photon energy (eV). Moreover, the calculated values of the lattice thermal conductivity are 12.26 (3.47)  $Wm^{-1}K^{-1}$  for SnTiO<sub>3</sub> at 300 K and (1100 K). We also found that the Seebeck coefficient and electrical conductivity yield fine values to satisfy the criterion of good thermoelectric device performance with low thermal conductivity. At higher temperatures (500–1200 K), SnTiO<sub>3</sub> exhibits a higher power factor and figure of merit than at lower temperatures. The predicted *ZT* at room temperature and optical absorption demonstrate that the examined material is more suited to optical applications than thermoelectric ones.

Author Contributions: Conceptualization, D.B., I.S., M.M., S.K.M. and R.S.; methodology, D.B., I.S., M.M. and R.S.; validation and formal analysis D.B., I.S., M.M. and R.S. resources, D.B. and M.M.S.; data curation, D.B. and M.M.S.; visualization, M.M.S. and M.M.; investigation, all authors; writing—original draft preparation, D.B., I.S., M.M. and S.K.M.; writing—review and editing, R.S. and M.M.S.; supervision, R.S. and M.M.S. All authors have read and agreed to the published version of the manuscript.

Funding: This research received no external funding.

**Data Availability Statement:** No new data were created or analyzed in this study. Data sharing does not apply to this article.

Conflicts of Interest: The authors declare no conflict of interest.

## References

- Im, J.-H.; Lee, C.-R.; Lee, J.-W.; Park, S.-W.; Park, N.-G. 6.5% Efficient Perovskite Quantum-Dot-Sensitized Solar Cell. *Nanoscale* 2011, 3, 4088–4093. [CrossRef]
- Manzoor, M.; Behera, D.; Sharma, R.; Iqbal, M.W.; Mukherjee, S.K.; Khenata, R.; Alarfaji, S.S.; Alzahrani, H.A. Investigation of the Structural, Mechanical, Optoelectronic and, Thermoelectric Characteristics of Cubic GeTiO<sub>3</sub>: An Ab Initio Study. *Mater. Today Commun.* 2023, 34, 105053. [CrossRef]
- Moon, S.-J.; Itzhaik, Y.; Yum, J.-H.; Zakeeruddin, S.M.; Hodes, G.; Grätzel, M. Sb2S3-Based Mesoscopic Solar Cell Using an Organic Hole Conductor. J. Phys. Chem. Lett. 2010, 1, 1524–1527. [CrossRef]
- 4. Taib, M.F.M.; Yaakob, M.K.; Badrudin, F.W.; Kudin, T.I.T.; Hassan, O.H.; Yahya, M.Z.A. First Principles Calculation of Tetragonal (P4 Mm) Pb-Free Ferroelectric Oxide of SnTiO<sub>3</sub>. *Ferroelectrics* **2014**, *459*, 134–142. [CrossRef]
- Akkerman, Q.A.; Gandini, M.; Di Stasio, F.; Rastogi, P.; Palazon, F.; Bertoni, G.; Ball, J.M.; Prato, M.; Petrozza, A.; Manna, L. Strongly Emissive Perovskite Nanocrystal Inks for High-Voltage Solar Cells. *Nat. Energy* 2016, 2, 16194. [CrossRef]
- Eperon, G.E.; Paternò, G.M.; Sutton, R.J.; Zampetti, A.; Haghighirad, A.A.; Cacialli, F.; Snaith, H.J. Inorganic Caesium Lead Iodide Perovskite Solar Cells. J. Mater. Chem. A 2015, 3, 19688–19695. [CrossRef]
- 7. Behera, D.; Mukherjee, S.K. Structural, Elastic, Electronic and Thermoelectric Properties of K2GeBr6: A First Principle Approach. *Mater. Today Proc.* 2023, *in press.* [CrossRef]
- Prado-Gonjal, J.; Lopez, C.A.; Pinacca, R.M.; Serrano-Sánchez, F.; Nemes, N.M.; Dura, O.J.; Martínez, J.L.; Fernández-Díaz, M.T.; Alonso, J.A. Correlation between Crystal Structure and Thermoelectric Properties of Sr1– XTi0. 9Nb0. 1O3– δ Ceramics. *Crystals* 2020, 10, 100. [CrossRef]
- 9. Piskunov, S.; Heifets, E.; Eglitis, R.I.; Borstel, G. Bulk Properties and Electronic Structure of SrTiO3, BaTiO3, PbTiO3 Perovskites: An Ab Initio HF/DFT Study. *Comput. Mater. Sci.* 2004, 29, 165–178. [CrossRef]
- 10. Cohen, R.E.; Krakauer, H. Electronic Structure Studies of the Differences in Ferroelectric Behavior of BaTiO<sub>3</sub> and PbTiO<sub>3</sub>. *Ferroelectrics* **1992**, *136*, 65–83. [CrossRef]
- Sághi-Szabó, G.; Cohen, R.E.; Krakauer, H. First-Principles Study of Piezoelectricity in PbTiO<sub>3</sub>. Phys. Rev. Lett. 1998, 80, 4321. [CrossRef]
- Saghi-Szabo, G.; Cohen, R.E.; Krakauer, H. First-Principles Study of Piezoelectricity in Tetragonal PbTiO<sub>3</sub> and PbZr 1/2 Ti 1/2 O 3. *Phys. Rev. B* 1999, 59, 12771. [CrossRef]
- 13. Rabe, K.M.; Ghosez, P. Ferroelectricity in PbTiO<sub>3</sub> Thin Films: A First Principles Approach. J. Electroceram. 2000, 4, 379–383. [CrossRef]
- 14. Meyer, B.; Padilla, J.; Vanderbilt, D. Theory of PbTiO<sub>3</sub>, BaTiO<sub>3</sub>, and SrTiO<sub>3</sub> Surfaces. *Faraday Discuss*. **1999**, *114*, 395–405. [CrossRef]
- 15. Wang, J.; Neaton, J.B.; Zheng, H.; Nagarajan, V.; Ogale, S.B.; Liu, B.; Viehland, D.; Vaithyanathan, V.; Schlom, D.G.; Waghmare, U. V Epitaxial BiFeO<sub>3</sub> Multiferroic Thin Film Heterostructures. *Science* **2003**, *299*, 1719–1722. [CrossRef] [PubMed]
- Yun, K.Y.; Ricinschi, D.; Kanashima, T.; Noda, M.; Okuyama, M. Giant Ferroelectric Polarization beyond 150 MC/Cm<sup>2</sup> in BiFeO<sub>3</sub> Thin Film. *Jpn. J. Appl. Phys.* 2004, 43, L647. [CrossRef]
- 17. Konishi, Y.; Ohsawa, M.; Yonezawa, Y.; Tanimura, Y.; Chikyow, T.; Wakisaka, T.; Koinuma, H.; Miyamoto, A.; Kubo, M.; Sasata, K. Possible Ferroelectricity in SnTiO<sub>3</sub> by First-Principles Calculations. *MRS Online Proc. Libr. (OPL)* **2002**, *748.* [CrossRef]

- Zhang, H.; Zhao, J.-T.; Grin, Y.; Wang, X.-J.; Tang, M.-B.; Man, Z.-Y.; Chen, H.-H.; Yang, X.-X. A New Type of Thermoelectric Material, Eu Zn<sub>2</sub>Sb<sub>2</sub>. J. Chem. Phys. 2008, 129, 164713. [CrossRef] [PubMed]
- Parker, W.D.; Rondinelli, J.M.; Nakhmanson, S.M. First-Principles Study of Misfit Strain-Stabilized Ferroelectric SnTiO<sub>3</sub>. *Phys. Rev. B* 2011, 84, 245126. [CrossRef]
- Hautier, G.; Jain, A.; Ong, S.P. From the Computer to the Laboratory: Materials Discovery and Design Using First-Principles Calculations. J. Mater. Sci. 2012, 47, 7317–7340. [CrossRef]
- 21. Hautier, G.; Fischer, C.C.; Jain, A.; Mueller, T.; Ceder, G. Finding Nature's Missing Ternary Oxide Compounds Using Machine Learning and Density Functional Theory. *Chem. Mater.* **2010**, *22*, 3762–3767. [CrossRef]
- Diehl, L.; Bette, S.; Pielnhofer, F.; Betzler, S.; Moudrakovski, I.; Ozin, G.A.; Dinnebier, R.; Lotsch, B. V Structure-Directing Lone Pairs: Synthesis and Structural Characterization of SnTiO<sub>3</sub>. *Chem. Mater.* 2018, 30, 8932–8938. [CrossRef]
- Pielnhofer, F.; Diehl, L.; Jiménez-Solano, A.; Bussmann-Holder, A.; Schön, J.C.; Lotsch, B. V Examination of Possible High-Pressure Candidates of SnTiO3: The Search for Novel Ferroelectric Materials. *APL Mater.* 2021, 9, 21103. [CrossRef]
- 24. de Lazaro, S.; Longo, E.; Sambrano, J.R.; Beltrán, A. Structural and Electronic Properties of PbTiO<sub>3</sub> Slabs: A DFT Periodic Study. *Surf. Sci.* 2004, 552, 149–159. [CrossRef]
- Matar, S.F.; Baraille, I.; Subramanian, M.A. First Principles Studies of SnTiO<sub>3</sub> Perovskite as Potential Environmentally Benign Ferroelectric Material. *Chem. Phys.* 2009, 355, 43–49. [CrossRef]
- Zhao, H.; Kimura, H.; Cheng, Z.; Wang, X.; Yao, Q.; Osada, M.; Li, B.; Nishida, T. A New Multiferroic Heterostructure of YMnO<sub>3</sub>/SnTiO<sub>3</sub>+ X. Scr. Mater. 2011, 65, 618–621. [CrossRef]
- 27. Hohenberg, P.; Kohn, W. Density Functional Theory (DFT). Phys. Rev. 1964, 136, B864. [CrossRef]
- Blaha, P.; Schwarz, K.; Madsen, G.K.H.; Kvasnicka, D.; Luitz, J. Wien2k. Augment. Plane Wave+ Local Orbitals Program Calc. Cryst. Prop. 2001, 60, 1–302.
- 29. Hybertsen, M.S.; Louie, S.G. First-Principles Theory of Quasiparticles: Calculation of Band Gaps in Semiconductors and Insulators. *Phys. Rev. Lett.* **1985**, *55*, 1418. [CrossRef]
- Perdew, J.P.; Burke, K.; Ernzerhof, M. Generalized Gradient Approximation Made Simple. *Phys. Rev. Lett.* 1996, 77, 3865. [CrossRef]
- 31. Perdew, J.P.; Ruzsinszky, A.; Csonka, G.I.; Vydrov, O.A.; Scuseria, G.E.; Constantin, L.A.; Zhou, X.; Burke, K. Restoring the Density-Gradient Expansion for Exchange in Solids and Surfaces. *Phys. Rev. Lett.* **2008**, *100*, 136406. [CrossRef]
- 32. Wu, Z.; Cohen, R.E. More Accurate Generalized Gradient Approximation for Solids. Phys. Rev. B 2006, 73, 235116. [CrossRef]
- 33. Monkhorst, H.J.; Pack, J.D. Special Points for Brillouin-Zone Integrations. *Phys. Rev. B* 1976, 13, 5188. [CrossRef]
- 34. Behera, D.; Abraham, J.A.; Sharma, R.; Mukerjee, S.K.; Jain, E. First Principles Study of New D0 Half-Metallic Ferromagnetism in CsBaC Ternary Half-Heusler Alloy. *J. Supercond. Nov. Magn.* **2022**, *35*, 3431–3437. [CrossRef]
- 35. Behera, D.; Manzoor, M.; Sharma, R.; Iqbal, M.W.; Mukherjee, S.K. First Principle Insight on Structural, Opto-Electronic and Transport Properties of Novel Zintl-Phase AMg<sub>2</sub>Bi<sub>2</sub> (A = Sr, Ba). *J. Solid State Chem.* **2023**, *320*, 123860. [CrossRef]
- Hafner, J. Materials Simulations Using VASP—A Quantum Perspective to Materials Science. Comput. Phys. Commun. 2007, 177, 6–13. [CrossRef]
- Dahbi, S.; Tahiri, N.; El Bounagui, O.; Ez-Zahraouy, H. Electronic, Optical, and Thermoelectric Properties of Perovskite BaTiO<sub>3</sub> Compound under the Effect of Compressive Strain. *Chem. Phys.* 2021, 544, 111105. [CrossRef]
- Johnston, K.; Huang, X.; Neaton, J.B.; Rabe, K.M. First-Principles Study of Symmetry Lowering and Polarization in Ba TiO<sub>3</sub>/SrTiO<sub>3</sub> Superlattices with in-Plane Expansion. *Phys. Rev. B* 2005, *71*, 100103. [CrossRef]
- 39. Murnaghan, F.D. The Compressibility of Media under Extreme Pressures. Proc. Natl. Acad. Sci. USA 1944, 30, 244–247. [CrossRef]
- Pielnhofer, F.; Diehl, L.; Jiménez-Solano, A.; Bußmann-Holder, A.; Christian, J.; Schön, B.V.L. 3. Examining Experimentally Accessible Structural Candidates of SnTiO3: The Search for Novel Ferroelectric Materials. In SnTiO3–A Lone Pair Model System for Studying Structure-Property Relationships in Photocatalysis, Ferroelectricity and Beyond; Ludwig-Maximilians-Universität München: Munich, Germany, 2020; Volume 44.
- Taib, M.F.M.; Yaakob, M.K.; Chandra, A.; Arof, A.K.M.; Yahya, M.Z.A. Effect of Pressure on Structural, Electronic and Elastic Properties of Cubic (Pm3m) SnTiO3 Using First Principle Calculation. *Adv. Mater. Res.* 2012, 501, 342–346.
- Wang, J.J.; Meng, F.Y.; Ma, X.Q.; Xu, M.X.; Chen, L.Q. Lattice, Elastic, Polarization, and Electrostrictive Properties of BaTiO<sub>3</sub> from First-Principles. J. Appl. Phys. 2010, 108, 34107. [CrossRef]
- 43. Taib, M.F.M.; Yaakob, M.K.; Hassan, O.H.; Chandra, A.; Arof, A.K.; Yahya, M.Z.A. First Principles Calculation on Structural and Lattice Dynamic of SnTiO<sub>3</sub> and SnZrO<sub>3</sub>. *Ceram. Int.* **2013**, *39*, S297–S300. [CrossRef]
- 44. Taib, M.F.M.; Yaakob, M.K.; Hassan, O.H.; Yahya, M.Z.A. Structural, Electronic, and Lattice Dynamics of PbTiO<sub>3</sub>, SnTiO<sub>3</sub>, and SnZrO<sub>3</sub>: A Comparative First-Principles Study. *Integr. Ferroelectr.* **2013**, *142*, 119–127. [CrossRef]
- Alam, N.N.; Malik, N.A.; Hussin, N.H.; Ali, A.M.M.; Hassan, O.H.; Yahya, M.Z.A.; Taib, M.F.M. First-Principles Study on Electronic Properties, Phase Stability and Strain Properties of Cubic (Pm3m) and Tetragonal (P4mm) ATiO3 (A = Pb, Sn). Int. J. Nanoelectron. Mater. 2020, 13.
- Behera, D.; Manzoor, M.; Mukherjee, S.K. Incorporation of Te in Enhancing Thermoelectric Response of AeAg2SeTe (Ae = Sr, Ba) Compounds: A DFT Insight. *Comput. Condens. Matter* 2022, 33, e00757. [CrossRef]
- 47. Gao, S.; Broux, T.; Fujii, S.; Tassel, C.; Yamamoto, K.; Xiao, Y.; Oikawa, I.; Takamura, H.; Ubukata, H.; Watanabe, Y. Hydride-Based Antiperovskites with Soft Anionic Sublattices as Fast Alkali Ionic Conductors. *Nat. Commun.* **2021**, *12*, 201. [CrossRef]

- Behera, D.; Manzoor, M.; Maharana, M.; Iqbal, M.W.; Zahid, T.; Lakra, S.; Mukherjee, S.K.; Alarfaji, S.S. Structural, Electronic, Optical, and Thermoelectric Response of Zintl Phase AAg2S2 (A = Sr/Ba) Compounds for Renewable Energy Applications. *Phys. B Condens. Matter* 2023, 649, 414446. [CrossRef]
- 49. Jamal, M.; Bilal, M.; Ahmad, I.; Jalali-Asadabadi, S. IRelast Package. J. Alloy. Compd. 2018, 735, 569–579. [CrossRef]
- 50. Grimvall, G. Thermophysical Properties of Materials; Elsevier: Amsterdam, The Netherlands, 1999; ISBN 0080542867.
- 51. Barsch, G.R. Adiabatic, Isothermal, and Intermediate Pressure Derivatives of the Elastic Constants for Cubic Symmetry. I. Basic Formulae. *Phys. Status Solidi* **1967**, *19*, 129–138. [CrossRef]
- 52. Behera, D.; Dixit, A.; Kumari, K.; Srivastava, A.; Sharma, R.; Mukherjee, S.K.; Khenata, R.; Boumaza, A.; Bin-Omran, S. Structural, Elastic, Mechanical, and Thermodynamic Characteristic of NaReO3 and KReO3 Perovskite Oxides from First Principles Study. *Eur. Phys. J. Plus* **2022**, 137, 1345. [CrossRef]
- 53. Bahera, D.; Dixit, A.; Nahak, B.; Srivastava, A.; Dubey, S.; Sharma, R.; Mishra, A.K.; Mukeerjee, S.K. Structural, Electronic, Elastic, Vibrational and Thermodynamic Properties of Antiperovskites Mg3NX (X = Ge, Sn): A DFT Study. *Phys. Lett. A* 2022, 453, 128478. [CrossRef]
- 54. Eglitis, R.I.; Piskunov, S.; Popov, A.I.; Purans, J.; Bocharov, D.; Jia, R. Systematic Trends in Hybrid-DFT Computations of BaTiO<sub>3</sub>/SrTiO<sub>3</sub>, PbTiO<sub>3</sub>/SrTiO<sub>3</sub> and PbZrO<sub>3</sub>/SrZrO<sub>3</sub> (001) Hetero Structures. *Condens. Matter* **2022**, *7*, 70. [CrossRef]
- 55. Eglitis, R.I.; Purans, J.; Popov, A.I.; Bocharov, D.; Chekhovska, A.; Jia, R. Ab Initio Computations of O and AO as Well as ReO2, WO2 and BO2-Terminated ReO<sub>3</sub>, WO<sub>3</sub>, BaTiO<sub>3</sub>, SrTiO<sub>3</sub> and BaZrO<sub>3</sub> (001) Surfaces. *Symmetry* **2022**, *14*, 1050. [CrossRef]
- Manzoor, M.; Chowdhury, S.; Sharma, R.; Iqbal, M.W.; Mukherjee, S.K.; Alarfaji, S.S.; Alzahrani, H.A. Insight on the Lattice Dynamics, Thermodynamic and Thermoelectric Properties of CdYF3 Perovskite: A DFT Study. *Comput. Theor. Chem.* 2022, 1217, 113928. [CrossRef]
- 57. Behera, D.; Mukherjee, S.K. Theoretical Investigation of the Lead-Free K2InBiX6 (X = Cl, Br) Double Perovskite Compounds Using First Principle Calculation. *JETP Lett.* **2022**, *116*, 537–546. [CrossRef]
- Taib, M.F.M.; Yaakob, M.K.; Badrudin, F.W.; Rasiman, M.S.A.; Kudin, T.I.T.; Hassan, O.H.; Yahya, M.Z.A. First-Principles Comparative Study of the Electronic and Optical Properties of Tetragonal (P4mm) ATiO<sub>3</sub> (A = Pb, Sn, Ge). *Integr. Ferroelectr.* 2014, 155, 23–32. [CrossRef]
- 59. Li, X.; Xia, C.; Wang, M.; Wu, Y.; Chen, D. First-Principles Investigation of Structural, Electronic and Elastic Properties of HFX (X = Os, Ir and Pt) Compounds. *Metals* 2017, 7, 317. [CrossRef]
- 60. Behera, D.; Sharma, R.; Ullah, H.; Waheed, H.S.; Mukherjee, S.K. Electronic, Optical, and Thermoelectric Investigations of Zintl Phase AAg2Se2 (A= Sr, Ba) Compounds: A First First-Principles Approach. *J. Solid State Chem.* **2022**, 132, 123259. [CrossRef]
- 61. Karki, B.B.; Wentzcovitch, R.M.; De Gironcoli, S.; Baroni, S. High-Pressure Lattice Dynamics and Thermoelasticity of MgO. *Phys. Rev. B* 2000, *61*, 8793. [CrossRef]
- 62. Behera, D.; Manzoor, M.; Iqbal, M.W.; Lakra, S.; Mukherjee, S.K. Revealing Excellent Electronic, Optical, and Thermoelectric Behavior of EU Based Euag2y2 (Y = S/Se): For Solar Cell Applications. *Comput. Condens. Matter* **2022**, *32*, e00723. [CrossRef]
- 63. Andritsos, E.I.; Zarkadoula, E.; Phillips, A.E.; Dove, M.T.; Walker, C.J.; Brazhkin, V.V.; Trachenko, K. The Heat Capacity of Matter beyond the Dulong–Petit Value. *J. Phys. Condens. Matter* 2013, *25*, 235401. [CrossRef] [PubMed]
- 64. Vajeeston, P.; Ravindran, P.; Fjellvåg, H. Prediction of Structural, Lattice Dynamical, and Mechanical Properties of CaB 2. *RSC Adv.* 2012, *2*, 11687–11694. [CrossRef]
- Yaseen, M.; Butt, M.K.; Ashfaq, A.; Iqbal, J.; Almoneef, M.M.; Iqbal, M.; Murtaza, A.; Laref, A. Phase Transition and Thermoelectric Properties of Cubic KNbO<sub>3</sub> under Pressure: DFT Approach. J. Mater. Res. Technol. 2021, 11, 2106–2113. [CrossRef]
- Behram, R.B.; Iqbal, M.A.; Alay-e-Abbas, S.M.; Sajjad, M.; Yaseen, M.; Arshad, M.I.; Murtaza, G. Theoretical Investigation of Mechanical, Optoelectronic and Thermoelectric Properties of BiGaO3 and BiInO3 Compounds. *Mater. Sci. Semicond. Process.* 2016, 41, 297–303. [CrossRef]
- Noor, N.A.; Hassan, M.; Rashid, M.; Alay-e-Abbas, S.M.; Laref, A. Systematic Study of Elastic, Electronic, Optical and Thermoelectric Properties of Cubic BiBO3 and BiAlO3 Compounds at Different Pressure by Using Ab-Initio Calculations. *Mater. Res. Bull.* 2018, 97, 436–443. [CrossRef]
- Ju, S.; Shiomi, J. Materials Informatics for Heat Transfer: Recent Progresses and Perspectives. *Nanoscale Microscale Thermophys.* Eng. 2019, 23, 157–172. [CrossRef]
- 69. Wood, C. Materials for Thermoelectric Energy Conversion. Rep. Prog. Phys. 1988, 51, 459. [CrossRef]
- Shah, S.H.; Khan, S.H.; Laref, A.; Murtaza, G. Optoelectronic and Transport Properties of LiBZ (B = Al, In, Ga and Z = Si, Ge, Sn) Semiconductors. J. Solid State Chem. 2018, 258, 800–808. [CrossRef]
- 71. Hoat, D.M. Electronic Structure and Thermoelectric Properties of Ta-Based Half-Heusler Compounds with 18 Valence Electrons. *Comput. Mater. Sci.* 2019, 159, 470–477. [CrossRef]
- 72. Anissa, B.; Radouan, D.; Benaouda, B. Optical and Thermoelectric Response of RhTiSb Half-Heusler. *Int. J. Mod. Phys. B* 2019, 33, 1950247. [CrossRef]
- Abraham, J.A.; Behera, D.; Kumari, K.; Srivastava, A.; Sharma, R.; Mukherjee, S.K. A Comprehensive DFT Analysis on Structural, Electronic, Optical, Thermoelectric, SLME Properties of New Double Perovskite Oxide Pb<sub>2</sub>ScBiO<sub>6</sub>. *Chem. Phys. Lett.* 2022, 806, 139987. [CrossRef]
- Haq, B.U.; AlFaify, S.; Laref, A.; Ahmed, R.; Butt, F.K.; Chaudhry, A.R.; Rehman, S.U.; Mahmood, Q. Optoelectronic Properties of New Direct Bandgap Polymorphs of Single-Layered Germanium Sulfide. *Ceram. Int.* 2019, 45, 18073–18078. [CrossRef]

- 75. Behera, D.; Mukherjee, S.K. Optoelectronics and Transport Phenomena in Rb<sub>2</sub>InBiX<sub>6</sub> (X = Cl, Br) Compounds for Renewable Energy Applications: A DFT Insight. *Chemistry* **2022**, *4*, 1044–1059. [CrossRef]
- 76. Noor, N.A.; Mahmood, Q.; Rashid, M.; Haq, B.U.; Laref, A.; Ahmad, S.A. Ab-Initio Study of Thermodynamic Stability, Thermoelectric and Optical Properties of Perovskites ATiO<sub>3</sub> (A = Pb, Sn). *J. Solid State Chem.* **2018**, *263*, 115–122. [CrossRef]
- 77. Zhu, H.; Zhao, T.; Zhang, B.; An, Z.; Mao, S.; Wang, G.; Han, X.; Lu, X.; Zhang, J.; Zhou, X. Entropy Engineered Cubic N-Type AgBiSe2 Alloy with High Thermoelectric Performance in Fully Extended Operating Temperature Range. *Adv. Energy Mater.* 2021, 11, 2003304. [CrossRef]
- 78. Manzoor, M.; Bahera, D.; Sharma, R.; Tufail, F.; Iqbal, M.W.; Mukerjee, S.K. Investigated the Structural, Optoelectronic, Mechanical, and Thermoelectric Properties of Sr<sub>2</sub>BTaO<sub>6</sub> (B = Sb, Bi) for Solar Cell Applications. *Int. J. Energy Res.* 2022, 46, 23698–23714. [CrossRef]

**Disclaimer/Publisher's Note:** The statements, opinions and data contained in all publications are solely those of the individual author(s) and contributor(s) and not of MDPI and/or the editor(s). MDPI and/or the editor(s) disclaim responsibility for any injury to people or property resulting from any ideas, methods, instructions or products referred to in the content.