STRUCTURAL AND ELECTRONIC PROPERTIES OF BaTe AND SrTe: A FIRST PRINCIPLES STUDY

G. Subhashree

Student, PG Department of Physics,

Shrimathi Devkunvar Nanalal Bhatt Vaishnav College for Women

Email: g.subha21@gmail.com

ABSTRACT:

First principles calculations have been used to investigate the structural and electronic properties of Alkaline earth (AE) telluride (AE = Ba, Sr) at an equilibrium volume. These compounds form a closed-shell ionic system crystallized in the NaCl-type (B1) structure at an ambient condition. We have considered the pressure induced B1-B2 phase transition of BaTe and SrTe compounds. MT potential method within Density functional theory (DFT) have been adapted to perform the comparative study of Barium Telluride and Strontium Telluride. Exchange correlation energy optimization is used to compute the total energy with the Local density approximation (LDA). The total energy of the system completely depends on the volume. Equilibrium lattice parameter and Bulk modulus of AETe (AE = Ba, Sr) compounds are calculated by using Murnaghan equation of state studies and the results were found to be in satisfactory agreement with the available literature.

Keywords: Ab-initio calculations; Bulk modulus; Density of states; Semiconducting II-VI materials; Alkaline earth chalcogenides; Optical device.

INTRODUCTION

High pressure-induced structural phase transition in alkaline earth chalcogenides has been studied extensively because of its large technological applications in microelectronics, light emitting diodes, laser diodes and many more optical devices [1,2]. Most of the alkaline earth chalcogenides crystallize in six-fold coordinated NaCl type (B1) structure under normal conditions. These compounds undergo a high-pressure phase transformation to eight-fold coordinated CsCl-type (B2) structure [3, 4, 5]. Alkaline earth chalcogenides show metallisation behaviour together with a structural phase transition under high pressure. [6]. A main feature in the electronic bands of alkaline earth chalcogenides is that there is no evidence of d-electron in the valence band. Temperature dependent transport properties of strontium chalcogenides in two different phases provides interesting results in thermoelectric properties [7]. The hardness parameter and elastic constants of strontium

chalcogens have been well explored using two body potential model by Srivastava et al., [8]. The elastic properties of Barium chalcogenides have been studied using full potential method by Bouhemadou et al., [9].

The objective of the present paper is to compute structural and electronic properties of BaTe and SrTe under high pressure phase transition from B1 phase to B2 phase using muffin-tin potential method [10] by utilising the density functional theory within the local density approximation [11,12].

Computational details

The total energy and electronic structure calculation of Alkaline earth (AE) telluride (AE = Ba, Sr) compounds have been investigated through the first principles calculations by using the computational scheme offered by Anderson's tight binding linear muffin-tin orbital method with atomic sphere approximation (ASA) [12]. In this method, the electronic structure calculation is based on the density functional theory (DFT) within the local density approximation (LDA) [13]. Exchange and correlation contributions to both the atomic and crystalline potentials have been included through the von-Berth Hedin parametrisation scheme [13]. The tetrahedron method of Brillouin zone integration was used for Density of states (DOS) studies [14]. E and k convergence are also checked carefully. Equilibrium lattice parameter were calculated by computing the total energy after reducing the crystal volume from $1.2V_0$ to $0.8V_0$ where V_0 is the equilibrium volume. The computed electronic total energies for BaTe and SrTe compounds with respect to relative volume were fitted using Murnaghan equation of state [15] to obtain the ground state properties. The pressure and bulk modulus were obtained from the total energy derivatives.

RESULTS AND DISCUSSION

Structural properties

The equilibrium lattice parameter and bulk modulus of BaTe and SrTe compounds in both B1 and B2 phases have been computed by fitting and energy-volume curve which is shown in **figure 1a and 1b.** From the figure, it can be clearly observed that the minimum of all the curves defines the equilibrium cell volume. B1 phase of BaTe and SrTe are energetically more favourable than the B2 phase which confirms good stability of B1 phase than B2 phase. Calculated structural parameters are reported in **Table 1**. The Equilibrium lattice parameters from our results are found in good agreement with the earlier theoretical results.

The bulk modulus of the compounds in both the phases are calculated from the relation $B = -V \, dP/dV$ and the values are presented in **Table 1**. A reasonable increment of Bulk modulus can be observed from B1 to B2 phase.
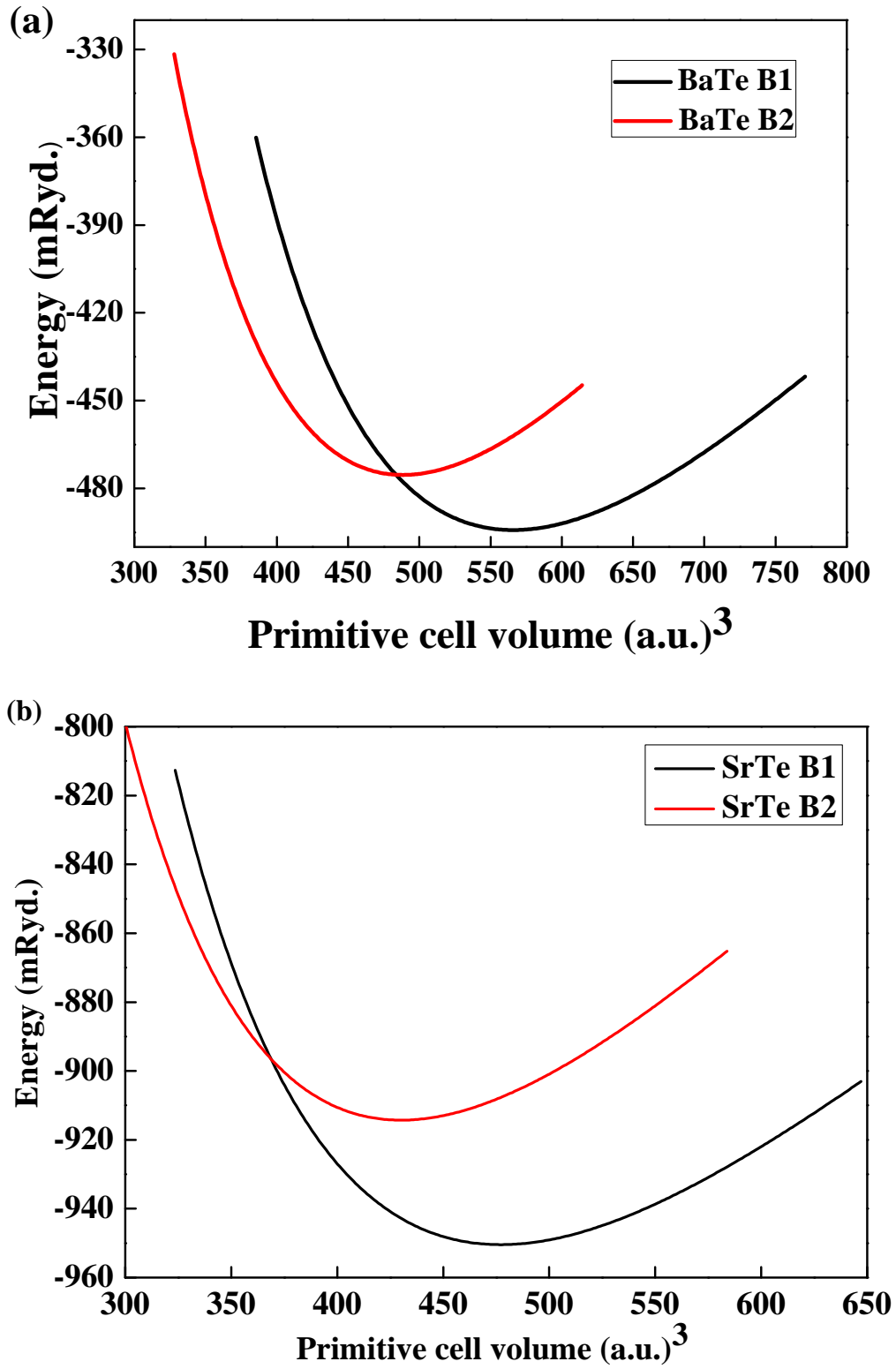
Figure 1: Variation of total energy as a function of cell volume for a)BaTe and b) SrTe in both the phases

Electronic properties

Figure 2 shows the self-consistent energy band structure along high symmetry directions of BaTe and SrTe in both the phases from the calculated equilibrium lattice constant. The overall band profiles are like each other. The gap around the fermi region confirms the semiconducting nature of the compounds. Band gap values are calculated for BaTe and SrTe in both the phases and the values are 3.12 eV, 1.63 eV, 3.40 eV and 1.23 eV, respectively. These are the band gap values of bulk AE Telluride material due to LDA. The reasonable decrement in the band gap can be well observed during the pressure induced phase transition for both compounds [3] [11]. The density of states plots confirms the same nature with bonding and antibonding regions for BaTe and SrTe in B1 and B2 phases.
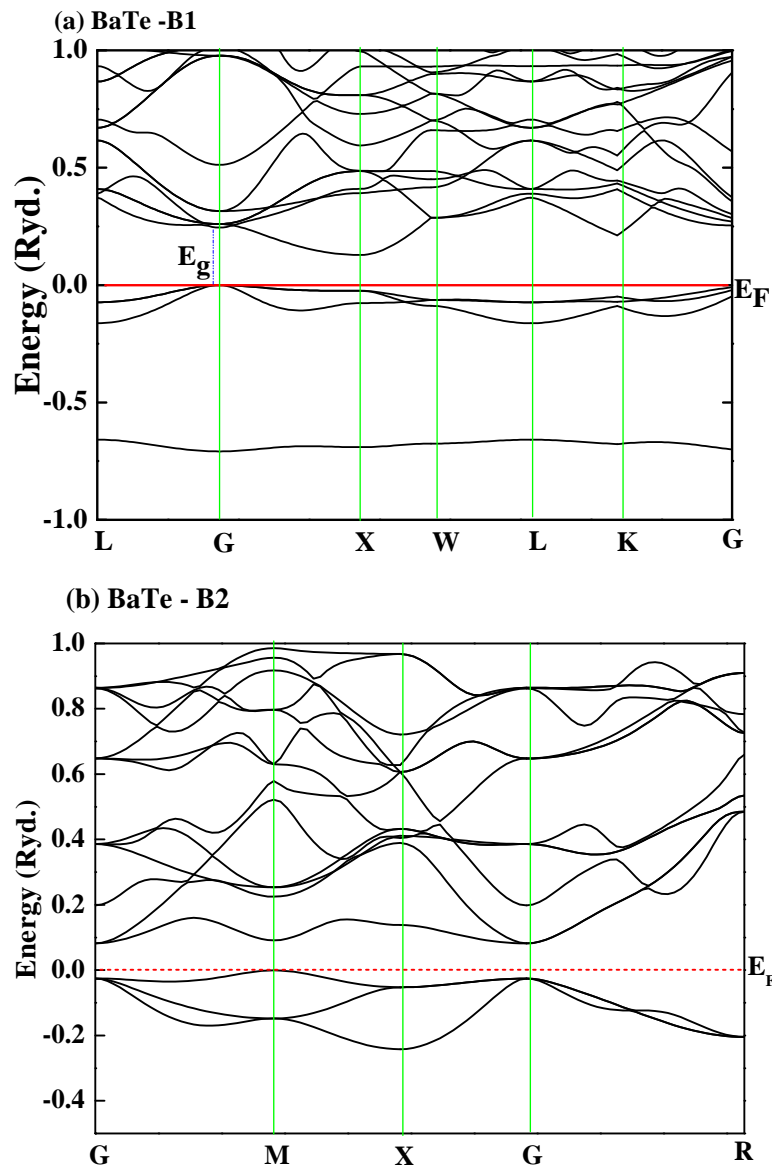

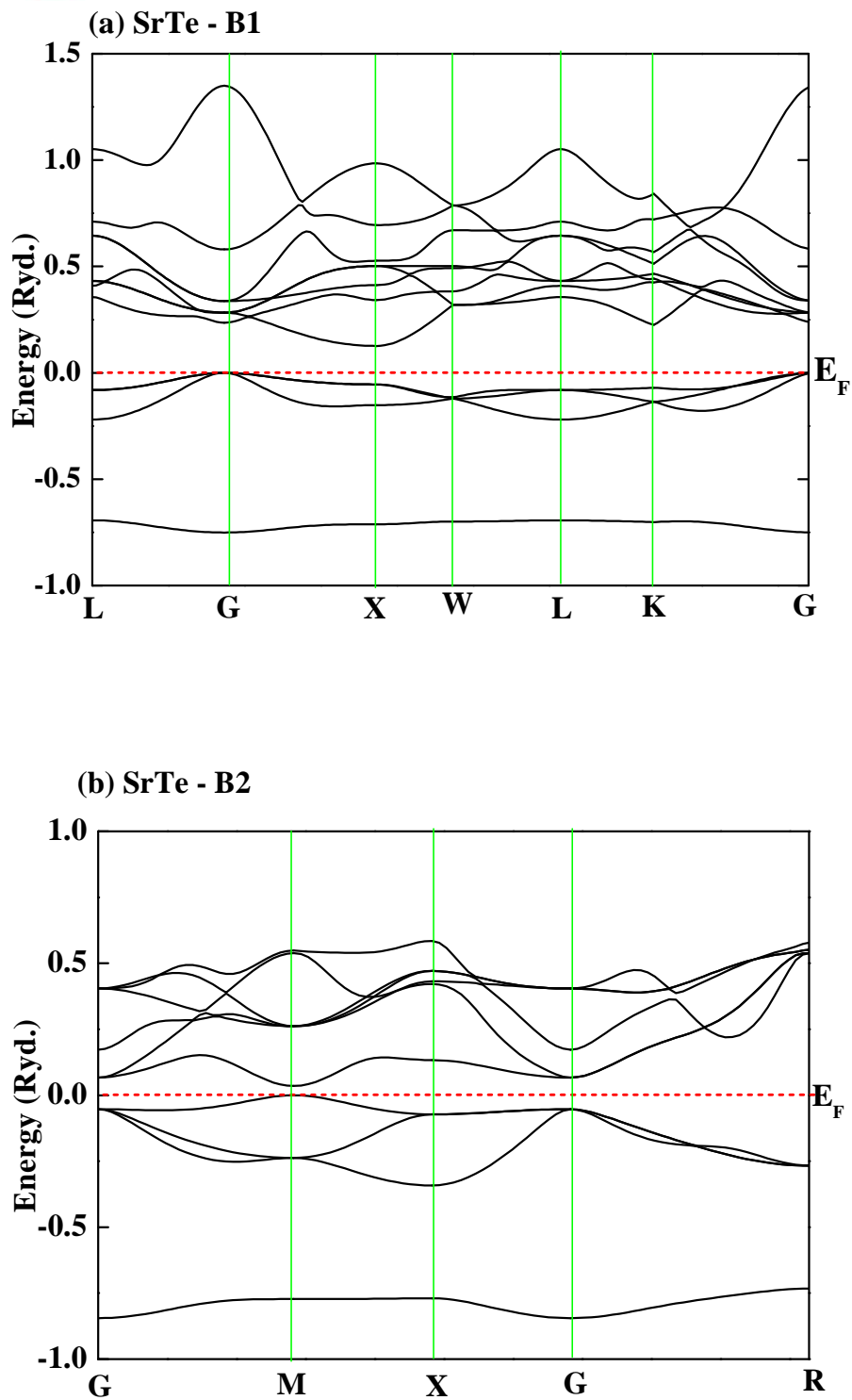**Figure 2: Band structure of BaTe along high symmetry directions in a) B1 phase b) B2 phase**

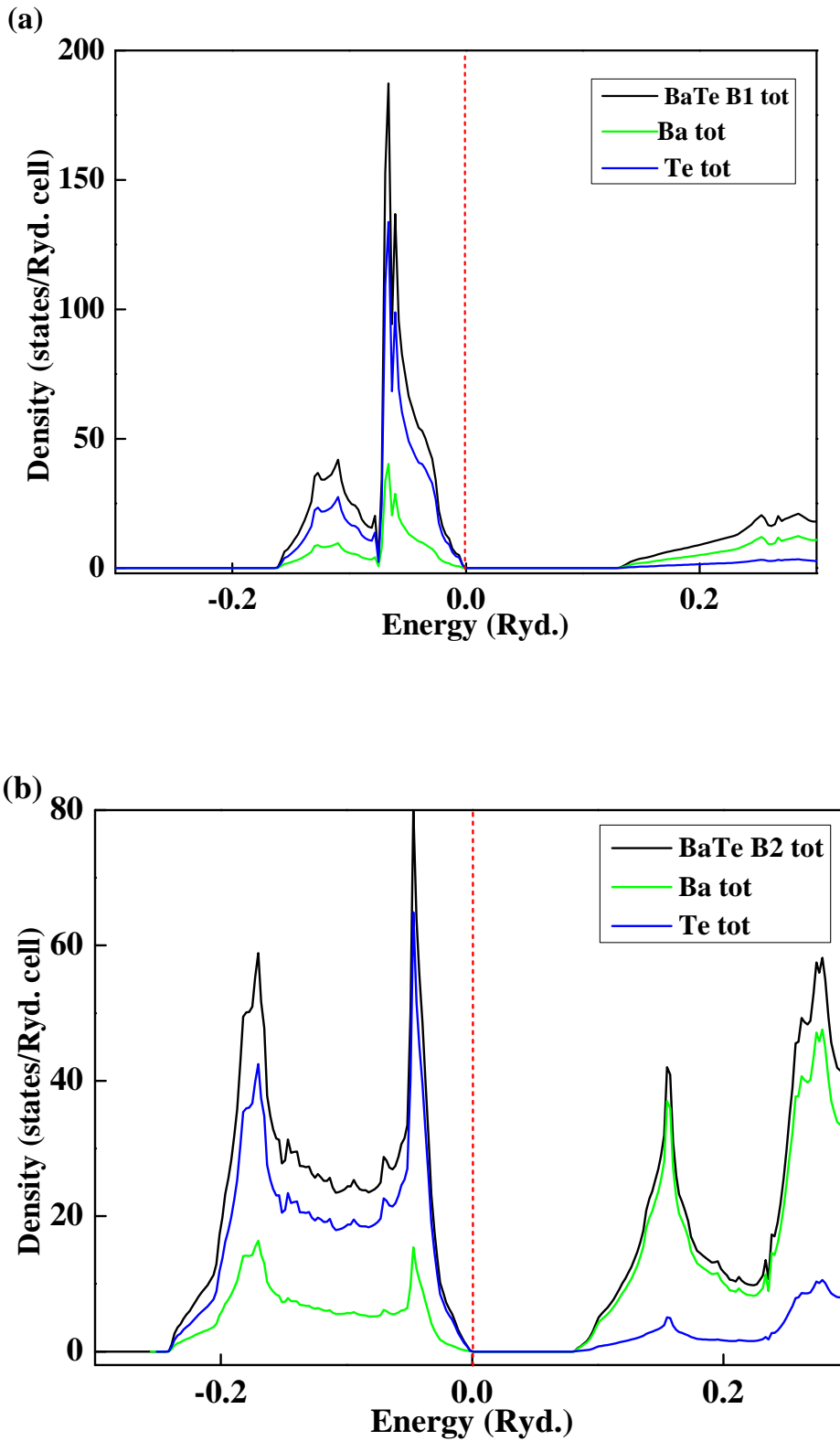**Figure 3: Band structure of SrTe along high symmetry directions in a) B1 phase b) B2 phase**

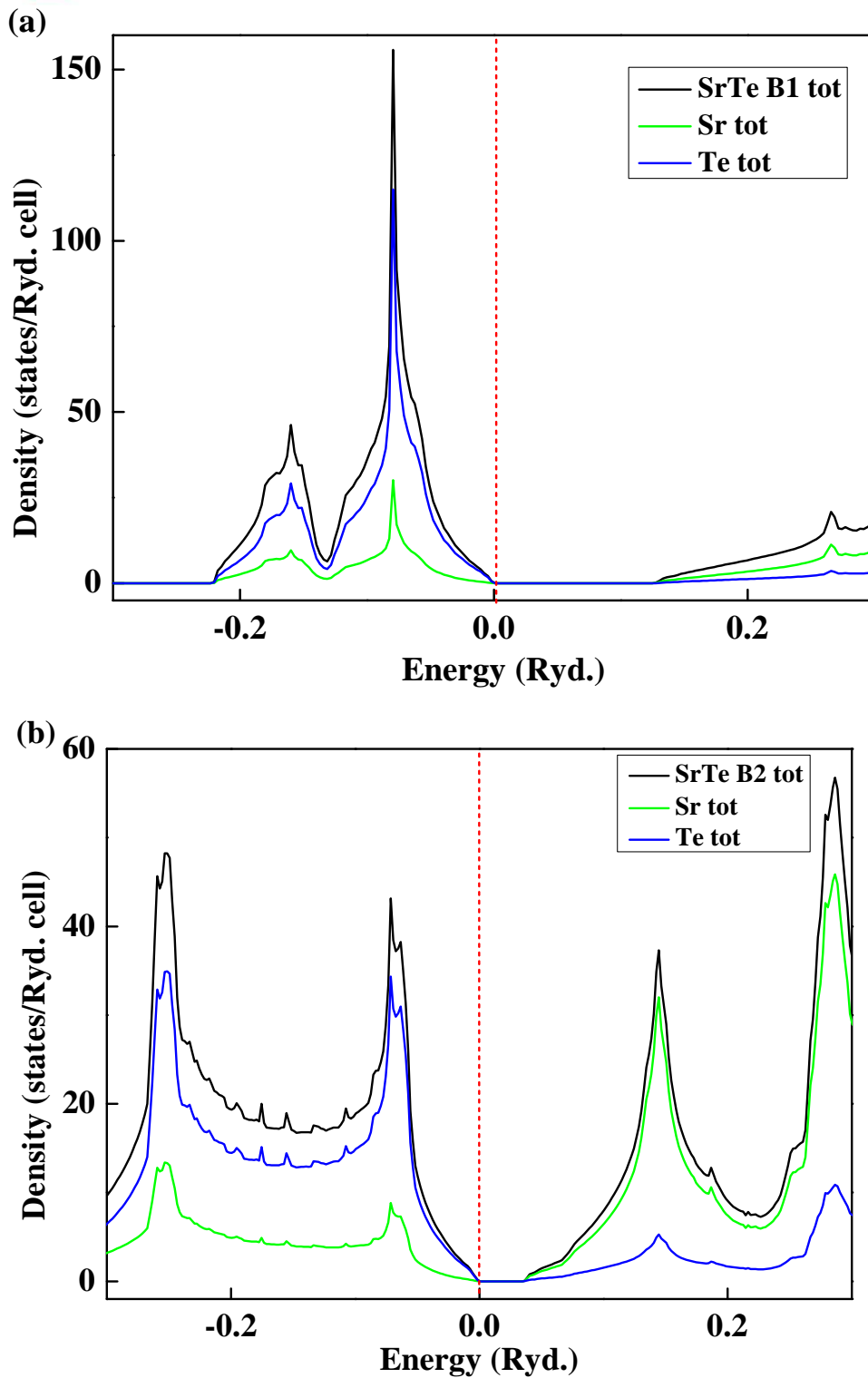**Figure 4: Density of states plot for BaTe in a) B1 phase and b) B2 phase**

Figure 5: Density of states plot for SrTe in a) B1 phase and b) B2 phase

Compounds	Phase	$a_0 (a.u.)$		$V_0 (a.u.)^3$		$B_0 (GPa)$		$S_0 (a.u.)$		$V_{trans} (a.u.)^3$		$p_{trans} (GPa)$		References
		Calc.	Ref.	Calc.	Ref.	Calc.	Ref.	Calc.	Ref.	Calc.	Ref.	Calc.	Ref.	
BaTe	B1	13.134	13.004[a]	566.47	539.0[i]	0.36	0.33[a,b]	5.13	-	484.01	-	3.68	4.16[i]	[a][4][b][17][i][16]
	B2	7.786	7.789[c]	488.56	464.1[i]	0.41	0.40[c] 0.39[f]	4.89	-					[c][9] [f][3][i][16]
SrTe	B1	12.40	12.69[d] 12.85[e]	476.67	465.3[i]	0.40	0.44[g] 0.39[e]	4.84	-	369.34	-	9.54	11.2[g] 12.5[j]	[d][7][e][19][g][11][i][16]
	B2	7.458	7.84[h]	430.09	419.0[i]	0.45	0.45[g] 0.42[e]	4.68	-					[e][19][g][11][h][20][i][16] [j][18]

Table 1: Calculated equilibrium lattice constant (a_0), equilibrium volume (V_0), Bulk modulus (B_0), Wigner-Seitz radius (S_0), Phase transition volume (V_{trans}), Phase transition pressure (p_{trans}).

CONCLUSION

The structural and electronic properties in Barium Telluride and Strontium Telluride of both B1 and B2 phases have been studied using tight binding linear muffin tin orbital method. The ground state structural properties have been obtained from the electronic total energy minimum and are found to be in good agreement. The structural phase stability in BaTe and SrTe compounds have been studied using the total energy calculations. The bulk moduli of both the phases are obtained from equilibrium lattice constant. The transition pressures were calculated are also in good agreement with existing results. From the electronic total energy versus volume curve, it has been found that B1 phase of BaTe and SrTe are energetically more favorable than B2 phase. The band gap values are also obtained from the band structure calculations. The band structure and DOS plots at Fermi level confirm the semiconducting nature of the material.

REFERENCES

1. Gokhan Gokoglu, Journal of Physics and Chemistry of Solids 69 (2008) 2924–2927.

2. Y. Nakanishi, T. Ito, Y. Hatanaka, G. Shiomaka Applied Surface Science 66 (1992) 515.

3. G. Kalpana, B. Palanivel , M. Rajagopalan, Physical Review B, 50 (1994) 17.

4. F. El. Haj Hassan and H. Akbarzadeh, Computational Material Science, 38 (2006) 362-368.

5. Manal M. Abdus Salam, DOI: https://doi.org/10.1016/j.cjph.2018.10.027.

6. Prafulla K. Jha, Umesh K. Sakalle, Sankar P. Sanyal, Journal of Physics and Chemistry of Solids, 59 (1998) 1633 – 1637.

7. Kaptan Rajput, Debesh R. Roy, Physica E, 119 (2020) 113965.

8. A. K. Srivastava, Noor Danish Ahrar Mundari, Computational Material Science 67(2013) 384-389.

9. A. Bouhemadou, Computational Material Science 38 (2008) 263-270.

10. O.K. Anderson and O. Jepsen, Physical Review Letters 53, 2571.

11. I. B. Shameem Banu, M. Rajagopalan, B. Palanivel, G. Kalpana and P. Shenbagaraman, Journal of low temperature of Physics, 112 (1998) 211-226.

12. H.L. Skriver, The LMTO Method, Springer, Berlin 1984.

13. Von Berth. U, Hedin. L, Journal of Physics, 5 (1972) 1629.

14. O. Jepsen and O.K. Anderson, Solid State Communication, 9 (1971) 1763.

15. Murnaghan. F. D., Proc. Natl.Sci. USA, 30 (1944) 5390.

16. Oliver Potzel, Gerhard Taubmann, Journal of Solid-State Chemistry, 184 (2011) 1079-1084.

17. T. A. Grzybowski, A. L. Ruoff, Physical Review Letters 53 (1984) 489.

18. Dinesh Varshney, N. Kaurav, R. Kinge, R.K. Singh, Computational Material Science, 41 (2008) 529-537.

19. H. G. Zimmer, H. Winzen and K. Syassen, Physical Review B, 32 (1985) 4066.

20. X. Zhou, J.C. Roehl, C. Lind, S.V. Khare, Journal of Physics: Condensed Matter 25 (2013) 075401.