



Research Article

First principles study of structural and electronic properties of binary strontium chalcogenides under pressure

Sofiane HAIRECHE^{1,2,*}, Abdenour BENMAKHOULF³, Mohamed BOUCHENAF^{4,5},
Said MAABED⁴, Mourad BOUHAMIDA⁴, Mohamed SIDOUMOU⁵

¹Laboratory of Physics of Experimental Techniques and Applications, University of Medea, Medea 26000, Algeria

²Laboratoire LASICOM, Faculté des Sciences, Université Saâd Dahlab de Blida, 09021, Algeria

³Laboratory for the Characterization and Valuation of Natural Resources, University of Bordj Bou Arreridj, 34000, Algeria

⁴Department of Material Sciences, Faculty of Science, Amar Telidji University, BP 37G, Laghouat, 03000, Algeria

⁵Theoretical Physics and Radiation Matter Interaction Laboratory (LPTHIRM) -Physics Department-University of Blida 1, 09000, Algeria

ARTICLE INFO

Article history

Received: 10 December 2021

Revised: 25 April 2022

Accepted: 06 June 2022

Keywords:

II-VI Semiconductors;
Strontium Chalcogenides;
Transition Pressure;
Metallization Pressure; DFT

ABSTRACT

The effect of pressure on the structural and electronic properties of the two binary compounds SrSe and SrTe have been investigated in the present work. The calculations were carried out with the CASTEP code which uses the density functional theory (DFT) based on the pseudopotential and plane-wave (PW-PP) method. To evaluate the exchange and correlation energy, we used the generalized gradient approximation (GGA-PBE). Our results show that, at ambient conditions, the two studied compounds are more stable in the NaCl-type phase (B1). Under the effect of pressure, the two materials undergo a phase transition to crystallize in the CsCl-like structure (B2) at pressures equal to 16 GPa and 12.33 GPa for the compounds SrSe and SrTe, respectively. Analysis of the band structure under conditions of pressure and zero temperature shows that the two compounds are indirect semiconductors. Under the effect of pressure, our calculations predict that the two compounds change electronically to become metals at pressures greater than 46 GPa for SrSe and 13 GPa for SrTe. To give a quantitative description of the variation of the structural and electronic parameters of the two structures with the pressure, we extracted the parametric functions of these parameters as a function of the pressure. Our results are presented and compared with a different experimental and theoretical works.

Cite this article as: Haireche S, Benmakhlouf A, Bouchenafa M, Maabed S, Bouhamida M, Sidoumou M. First principles study of structural and electronic properties of binary strontium chalcogenides under pressure. Sigma J Eng Nat Sci 2023;41(6):1231–1242.

*Corresponding author.

*E-mail address: shaireche@outlook.fr

This paper was recommended for publication in revised form by
Regional Editor Ahmet Selim Dalkilic



INTRODUCTION

II-VI semiconductors, commonly known as alkaline-earth chalcogenides, have become the subject of study in several experimental and theoretical research studies in recent decades [1-5]. Historically, strontium chalcogenides SrX (X=O, S, Se Te) emerged in the late 1970's. The research of Ellervee (1977), Asano et al. (1978, 1983), Asano and Yamashita (1981, 1983), Yamashita et al. (1984), and Baby and Nampoori (1992) is considered to be one of the pioneering works. These studies primarily focused on the structural features of all these materials [6-8]. In 1985, Zimmer et al. experimentally investigated the effect of pressure on the structural properties of the SrTe compound [9]. In 1994, Luo et al. estimated an upper limit of about 55 GPa for the metallization of the SrSe compound [10]. The optical and chemical properties of some chalcogenides had been studied by Kaneko et al. in 1982. Then, in 1988, from a study on the optical properties of high-quality monocrystals, Kaneko et al. estimated a direct gap of 4.47 eV and an indirect gap of 3.81 eV for SrSe [11-12].

The both compounds SrSe and SrTe possess various functional properties which can be exploited in optoelectronic and spintronic devices, namely in long wavelength imaging applications of infrared diode lasers or photovoltaic energy converters [3]. These compounds are used as potential components in several technological devices such as medical diagnostics, industrial process control and air pollution monitoring [4,13]. Additionally, these compounds have been successfully used in infrared sensors, in light emitting devices and as infrared lasers in optical fibers, as thermoelectric materials, in solar panels, and in window coverings [5,14]. Generally, the binary compounds based on strontium such as SrSe and SrTe crystallize in the NaCl phase at zero pressure and temperature conditions. Under the effect of a hydrostatic pressure of about 14.2 GPa (12 GPa) for SrS (SrTe), a transition to the CsCl phase had been observed experimentally [10]. However, despite the abundant literature discussing the effect of hydrostatic pressure on the properties of these materials, very little is known about the evolution of structural and electronic properties as function of the pressure applied. In previous works, it was been found that the occurrence of the pressure-induced metallization is intimately linked to a structural phase transition [15]. Because of the deficiency of information on such an important topic, we theoretical study the evolution of the structural and electronic properties under pressure of the two compounds SrSe and SrTe in the two phases NaCl and CsCl. In addition, we want to know the behavior of the different electronic properties such as the energy band gap with respect to the phase change B1 -B2 and B2-metal. The pressure-induced manipulation of the transport properties of the two studied materials possibly will deliver crucial information towards their practical applications. Accordingly, the objective of this work is to achieve a better understanding of the structural and electronic properties of

SrX (X=Se, Te) under pressure and their phase transition. Moreover, we search for optimize the value of the pressure P_M with which, the two semiconductors become metals.

CALCULATION DETAILS

First-principles calculations were performed within the context of the generalised gradient approximation (GGA) as implemented in the CASTEP code [16] and the pseudopotential and plane-wave approach (PP_PW) of density functional theory (DFT) [17]. The exchange–correlation energy was treated using the generalized gradient approximation (GGA) and the Perdew–Burke–Ernzerhof functional (PBE) [18]. The pseudo-potential of Vanderbilt-type ultra-soft was used to compute the potential seen by the valence electrons [19]. The choice of this potential allows to have the following valence configurations: ($4s^2 4p^6 5s^2$) for the Sr, ($4s^2 4p^4$) for the Se and ($5s^2 5p^4$) for the Te. Self-consistent calculations are considered to be converged when the total energy of the system is minimal [20]. Thus, we have chosen the following convergence tolerance criteria: a total energy difference less than 10^{-6} eV/atom, a maximum ionic strength of Hellmann-Feynman of 0.01 eV/Å, and a maximum displacement of 5×10^{-4} Å [21].

In an ab-initio calculation, it is necessary to test the convergence of the results with respect to the cut-off energy (E_{cut}) and the *K-points* mesh configuration in the first Brillouin zone (1BZ). According to the results presented in Figures 1 and 2, a good convergence is obtained for a plane-wave energy of $E_{cut-off}$ values of 700 eV and $8 \times 8 \times 8$ K-points mesh configuration.

PHYSICAL PROPERTIES OF SRSE AND SRTE COMPOUNDS AT ZERO PRESSURE

Structural Properties

The SrSe and SrTe compounds crystallize in the cubic structure in the two phases B1 of the space group $Fm\bar{3}m$ (N°.225) and B2 of the space group $Pm\bar{3}m$ (N°.221). In B1 phase (NaCl structure), the conventional unit cell has 4 atoms which occupy the Sr the positions (0,0,0); (0.5, 0.5, 0); (0.5, 0, 0.5); (0, 0.5, 0.5) and X element (X=Se, Te) (0.5, 0.5, 0.5); (0.5, 0, 0); (0, 0.5, 0) (0, 0, 0.5). In the second B2 phase (CsCl structure) the atoms in each unit cell are two atoms which occupy the positions Sr (0, 0, 0) and X (0.5, 0.5, 0.5). The conventional unit cells of B1 and B2 phases are illustrated in Figure 3.

To begin the geometric optimization of the studied compounds, we used the structural parameters obtained experimentally from the references [22-23]. The results of optimization of the lattice parameter a and the unit cell volume V at zero pressure are collected in Table 1 which also contains results of others calculations as well as experimental references. Our results for SrSe (SrTe) compound show a difference from experimental data less than 0.38%

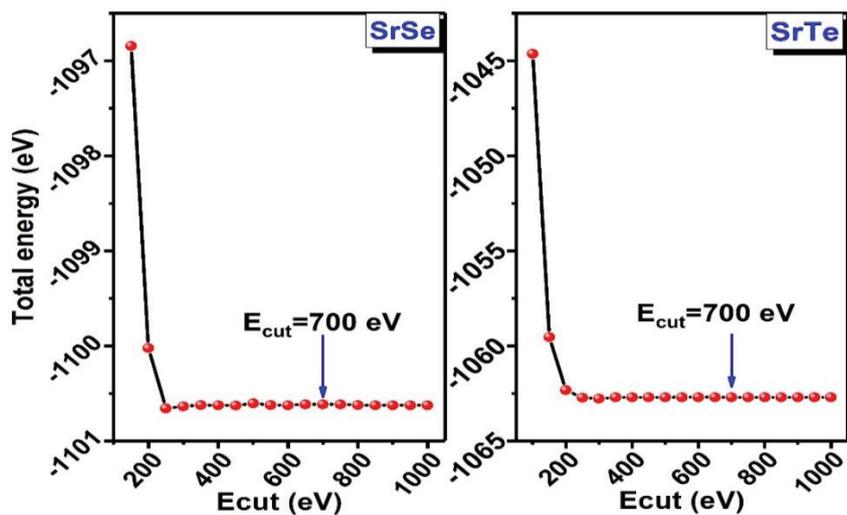


Figure 1. Convergence curve for total energy for SrS (B1) and SrTe(B1) in relation to cut-off energy.

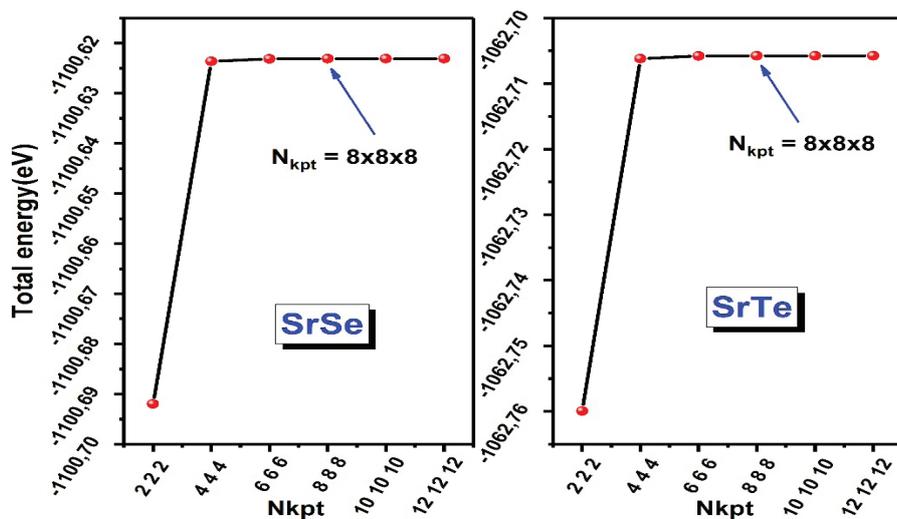


Figure 2. Convergence curve of the total energy for SrS (B1) and SrTe (B1) with respect to the k-point mesh in 1BZ.

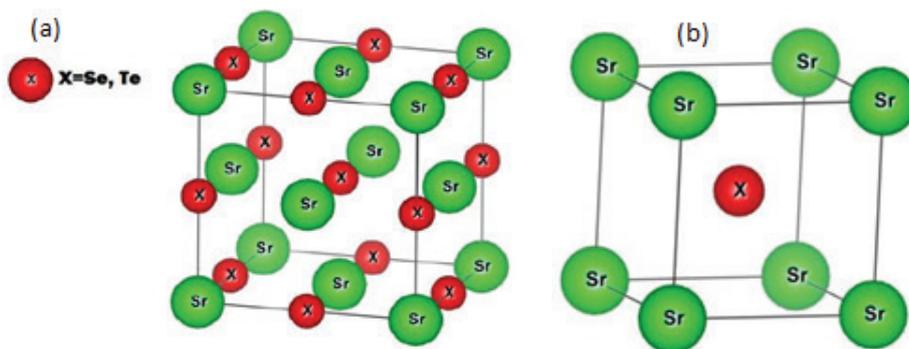


Figure 3. Crystal structure of compound SrX (X = Se, Te), (a) phase B1(NaCl), (b) phase B2(CsCl).

Table 1. Optimized cell volume V , lattice parameters a and the inter-atomic distances d for the SrSe and SrTe at zero pressure in phase B1

	SrSe			SrTe		
	a (Å)	V (Å ³)	Sr-Se bond	a (Å)	V (Å ³)	Sr-Te bond
Our results	6,254	244,60	3.127	6,719	303,33	3.360
Experimental data	6.234 ⁽¹⁾	242,27 ⁽¹⁾	3.118 ⁽¹⁾	6.659 ⁽²⁾	295,28 ⁽²⁾	3.330 ⁽²⁾
Other (theoretical)	6.29 ⁽³⁾	250,40 ⁽³⁾	3.870 ⁽³⁾	6.71 ⁽³⁾	302.11 ⁽³⁾	3.114 ⁽³⁾
	6.307 ⁽⁴⁾	250,88 ⁽⁴⁾	3.12 ⁽⁸⁾	6.572 ⁽⁵⁾	283.85 ⁽⁵⁾	3.24 ⁽⁸⁾
	6.300 ⁽⁶⁾	250,047 ⁽⁶⁾	-	6.718 ⁽⁶⁾	303 19 ⁽⁶⁾	-
	6.205 ⁽⁷⁾	238.90 ⁽⁷⁾	-	6.613 ⁽⁷⁾	289.19 ⁽⁷⁾	-
D (%)	0.32	0.96	0. 29	0.90	2.73	0.9

⁽¹⁾Ref.: [10]; ⁽²⁾Ref.: [9]; ⁽³⁾Ref.: [23]; ⁽⁴⁾Ref.: [3]; ⁽⁵⁾Ref.: [25]; ⁽⁶⁾Ref.: [13]; ⁽⁷⁾Ref.: [14]; ⁽⁸⁾Ref.: [26]

and 1.19% (0.88% and 2.68%) for the lattice parameter a and the cell volume V respectively. According to the criteria reported on the DFT (GGA) results given in reference [24], our results show good agreement with those given in experiments, which makes our following results more justified.

One of the basic methods for examining valence charge distributions and the types of chemical bonds that exist between the constituent atoms of a compound is the use of valence electronic charge density contour plots. From our calculations of the Mulliken population, we were able to determine the length and the nature of the Sr-X bond ($X = \text{Se, Te}$). According to the values in Table 1, One of the basic methods for examining valence charge distributions and the types of chemical bonds that exist between the constituent atoms of a compound is the use of valence electronic charge density contour plots. To qualitatively illustrate the nature of the bond between close neighbors, we have plotted, in figure 4, the two-dimensional charge density projected on the lattice planes (101) and (110) for SrSe and SrTe, respectively. We notice that an almost spherical charge density surrounds the two atoms Sr and Se. In the common region

between the two atoms Sr and Se shows a weak charge distribution, indicating the existence of a very weak covalent bond. With a slight variation in specifics, the SrTe molecule exhibits the identical effect.

Band Structures

We investigated the band structures of the two binary compounds SrSe and SrTe in the NaCl phase using the GGA approximation, with optimized lattice parameters. We have calculated the band structures for both SrSe and SrTe compounds and the results are plotted in Figure 5. The valence and the conduction bands are separated by a narrow zone of 2.30 eV for SrSe and 1.75 eV for SrTe. Additionally, it is noted that in both cases, the valence band maximum is at the point of high symmetry, or Γ , while the conduction band minimum is at point X. As a result, the two compounds are indirect gap semiconductors of type (Γ - X). Table 2 contains the different values of the gap calculated for the two structures, with the experimental and theoretical data available in the literature. It is well known that the theoretical gaps obtained by the GGA are approximately

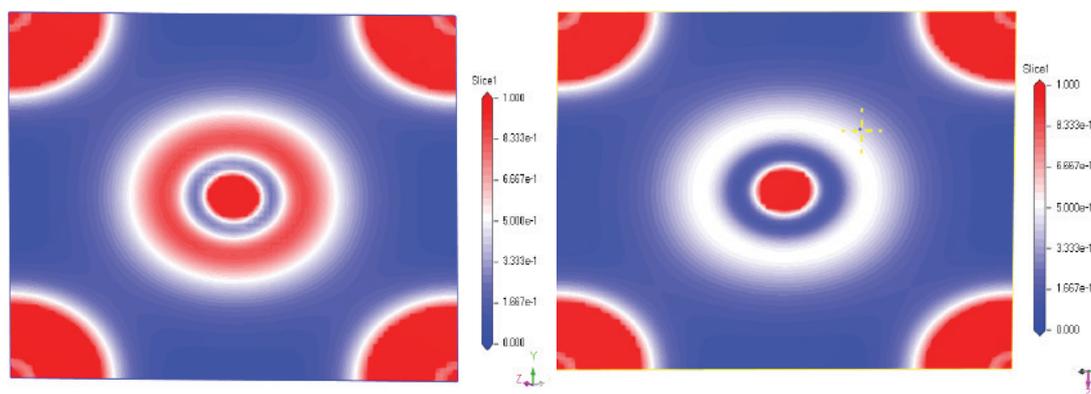


Figure 4. Contour plots of the charge density calculated with the GGA-PBE approximation for the two compounds, at zero pressure: (a) SrSe projected on (101), (b) SrTe projected on (110).

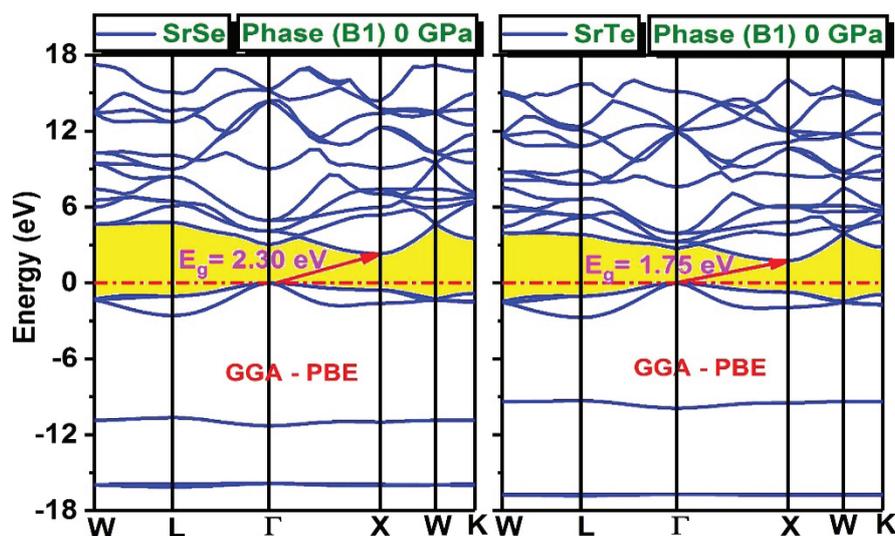


Figure 5. Band structures of the SrSe and SrTe compounds under ambient conditions. The basic band gap is shown by the darkened area.

Table 2. The direct (Γ - Γ) and indirect (Γ -X) gaps energy (eV) of SrSe and SrTe in phase B1 at zero pressure

	Gap direct (Γ - Γ)			Gap indirect (Γ -X)		
	Our results	Experimental	Other (theoretical)	Our results	Experimental	Other (theoretical)
SrSe	3.034	4.52 ^(1,2)	2.86 ⁽³⁾ 3.119 ⁽³⁾ 2.862 ⁽⁷⁾ 2.911 ⁽⁸⁾	2.30	3.81 ^(1,2)	2.13 ⁽³⁾ 2.137 ⁽⁴⁾ 2.216 ⁽³⁾ 2.232 ⁽⁷⁾ 3.377 ⁽⁸⁾
SrTe	2.73	3.6 ⁽¹⁾	2.93 ⁽³⁾ 2.7173 ⁽⁵⁾ 2.740 ⁽⁷⁾ 2.144 ⁽⁸⁾	1.75	2.9 ⁽³⁾ 3.813 ⁽⁶⁾	1.64 ⁽³⁾ 1.542 ⁽⁴⁾ 1.7747 ⁽⁵⁾ 1.760 ⁽⁷⁾ 2.665 ⁽⁸⁾

⁽¹⁾ Ref:[27]; ⁽²⁾ Ref: [28]; ⁽³⁾ Ref:[25]; ⁽⁴⁾ Ref:[29]; ⁽⁵⁾ Ref:[30]; ⁽⁶⁾ Ref:[11]; ⁽⁷⁾ Ref:[13]; ⁽⁸⁾ Ref:[14]

underestimated by 30% [24]. In the case of the two compounds studied, the values obtained by our calculations are lower than those given experimentally by approximately 39.5% and 39.6% for SrSe and SrTe, respectively. By comparing our results with the theoretical ones given in Table 2, we see an improvement in the value of the gap for SrSe.

Density of States (DOS)

We examined the total and partial density of states (TDOS and PDOS) for SrSe and SrTe compounds at zero pressure in order to verify the contribution of each atomic band inside the top of the valence band and the bottom of the conduction band. The origin of energies is generally

fixed at the Fermi level. The TDOS and PDOS for the two compounds are showed in Figure 6. The TDOS and the PDOS of the two materials SrSe and SrTe are similar with some differences in the details. Moreover, it can be seen that the TDOS can be divided into four distinct regions with respect to the energy for the two compounds. The first area is located between -20 eV and -15 eV. This area is due to the contribution of the p-states of the Sr and Se atoms to the SrSe compound and only the p-orbitals of the Sr atom in the SrTe compound. The second area is located between -8 eV and -12 eV. This area is dominated by the d-orbitals of the Se (Te) atoms for SrSe (SrTe) compounds. The following area is between -3.5 eV and the Fermi level at 0 eV. This

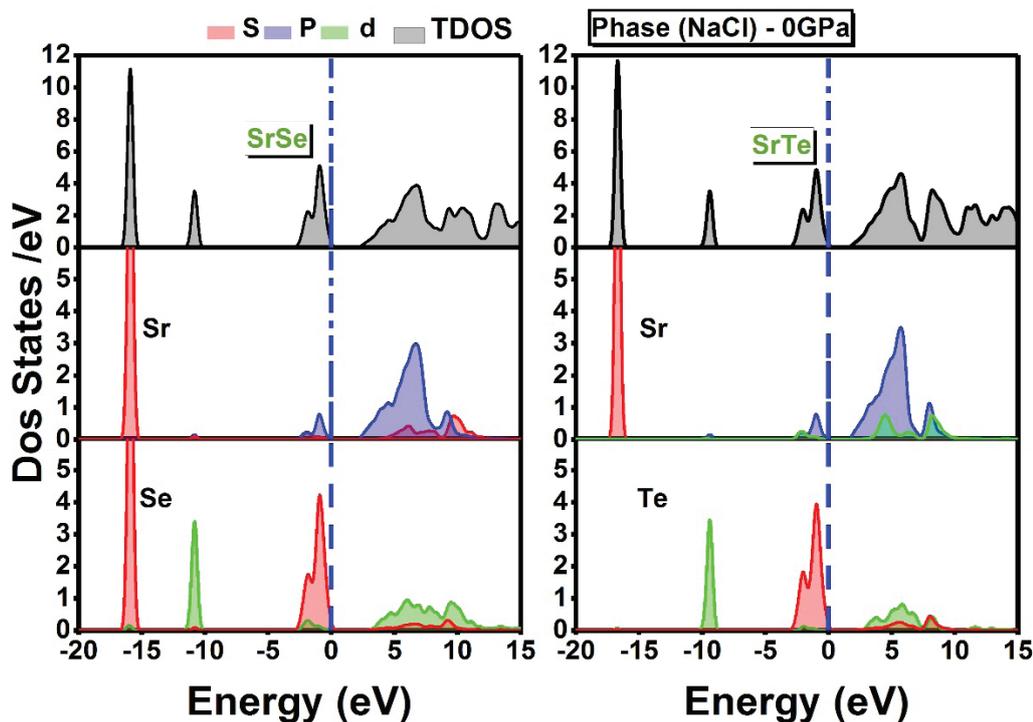


Figure 6. Projected and total density of states for the two compounds SrSe and SrTe in phase B1 at 0 GPa.

area is mainly due the p-orbitals for both Se and Te atoms, with a very small contribution from the s-orbitals of the Sr atom. The last area is between the Fermi level at 0 eV and 15.00 eV. For both compounds, this area is mostly derived from the d-orbitals of the Sr atom, with a little contribution from the s-orbital of the Sr atom. We note that the energy gap of the two compounds is located between a maximum energy of the valence band formed of the p-Sr states for the SrSe compound and of the p-Te states for the SrTe compound and a minimum of energy which essentially comes from the d-states of the Se atom for the two materials. The same behavior of total and partial density of state has been reported in previous works [3, 22, 25].

PHYSICAL PROPERTIES OF SRSE AND SRTE AS FUNCTION OF PRESSURE

Structural Properties

We investigate the structural characteristics under ambient and high-pressure settings in order to gain a microscopic understanding of the material properties. A solid undergoes a phase transition, or change in volume and symmetry, when hydrostatic pressure is applied to it. When a phase becomes unstable under specific thermodynamic circumstances, a phase transition occurs. The most stable phase corresponds, at zero temperature, to a minimum of the total energy, Gibbs energy $G = E + PV - TS$ where S denotes the entropy, or the enthalpy $H = E + PV$.

The internal energy will change throughout this transition, resulting in changes to the equilibrium parameters, including the lattice parameter a . In our simulations, we determine the structural stability of the two examined phases and the phase transition pressure, as the following: (i) we consider a two-phase system; B1 structure of NaCl type and B2 structure of CsCl type. (ii) First, we find the lowest of the total energy, Gibbs energy G , or enthalpy H for each value of the hydrostatic pressure P . The fact that the phase with the lowest enthalpy or Gibbs energy under typical circumstances will be the most stable phase justifies finding the minimum. Then we calculate the new value of lattice parameter corresponding to pressure P . (iii) The pressure value at which the two enthalpies of the two phases, B1 and B2, are equal is known as the transition pressure (P_t). In Figure 7 we plot the variation of enthalpy as a function of hydrostatic pressure. The most stable structure at zero pressure corresponds to phase B1 (NaCl). The transition to phase B2 (CsCl) takes place at a transition pressure P_t of the order of 16 GPa for SrSe and 12.33 GPa for SrTe.

In Table 3, we compare our obtained transition pressure with other theoretical [23] and experimental [9-10] data. We note that for the SrSe compound, the P_t value for pressure is greater than the values obtained experimentally [10], by M. Souadkia using the Hartwigsen–Goedecker–Hutter pseudopotential [23], and by R. Kheneta using the full-potential linearized augmented plane wave technique (FP-LAPW) [22]. On the other hand, for the case of the SrTe compound, we found a value of the transition pressure

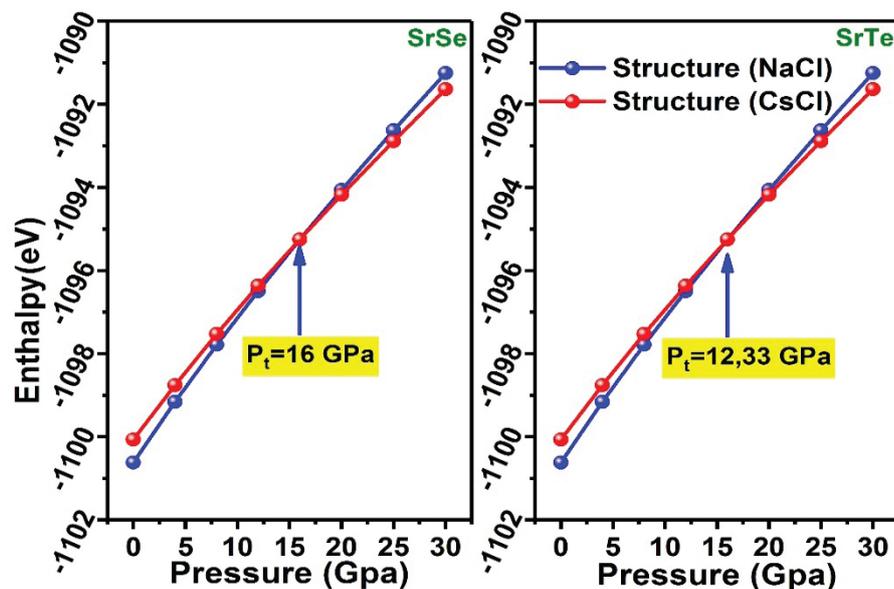


Figure 7. Enthalpy variation as function of pressure for the two compounds SrSe and SrTe.

Table 3. Transition pressure (in GPa) of the two compounds SrSe and SrTe calculated (Cal.) In comparison with other work (others)

Transition	Pt			
	Cal	Exp	Others	ΔP %
SrSe	16	14 ⁽¹⁾	13.6 ⁽³⁾ 15.55 ⁽⁴⁾ 14.5 ⁽⁵⁾	14.28
SrTe	12.33	12.0 ⁽¹⁾ 12.0 ⁽²⁾	12.3 ⁽³⁾ 13.24 ⁽⁶⁾	2.75 -

⁽¹⁾Ref:[10]; ⁽²⁾Ref:[9]; ⁽³⁾Ref:[23]; ⁽⁴⁾Ref:[3]; ⁽⁵⁾Ref:[22] ⁽⁶⁾Ref:[20]

compared to other theoretical [20, 23] and experimental work [9, 10]. It's also noteworthy to see that when the chalcogen's atomic number increases from Se to Sr, the computed transition pressure lowers.

There is good agreement between these values and previous theoretical studies as well as experimental results.

Plotting the two compounds' variations in volume V and lattice parameter a versus hydrostatic pressure between 0 and 30 GPa is done. Figure 8 shows that for both materials and both phases, the lattice parameter falls as pressure increases. Thus, for the four cases under study, this is followed with a decrease in volume. We plot the two parameters, a and V , as a function of pressure P (see Figure 8) to get a quantitative description of their change. Next, we identify a quadratic least squares fitting function that has the following form:

$$a(P) = y_0 + y_1 \cdot P + y_2 \cdot P^2 \quad (1)$$

$$V(P) = x_0 + x_1 \cdot P + x_2 \cdot P^2 \quad (2)$$

Table 4 displays the values of the linear and quadratic coefficients for the lattice parameters for SrSe and SrTe as a function of pressure.

In order to quantitatively study the phase transition behavior of the two compounds under scrutiny, we plot the relative variations of the lattice parameters a/a_0 and of the volume V/V_0 as a function of the pressure, see Figure 9.

The parameters a_0 and V_0 are the values of the lattice parameter and of the unit cell volume at zero pressure, successively. The results of the linear fit of these graphs are listed in Table 5.

From these data, we observe a decrease of the lattice parameter for both compounds SrSe and SrTe in each phase. In the same compound, it is noticed that the variation of the lattice parameter a in phase B1 is faster than that of phase B2.

Electronic Properties

In this part, we examine how pressure acting in a range of 0 to 30 GPa affects the electronic characteristics of the binary semiconductor compounds SrSe and SrTe.

In order to ensure phase B2 stability, it is important to investigate the electronic structure of materials under the influence of hydrostatic pressure. The band structures computed for the two compounds, SrSe and SrTe, under pressures of 16.5 GPa and 12.5 GPa, respectively, are shown in Figure 10.

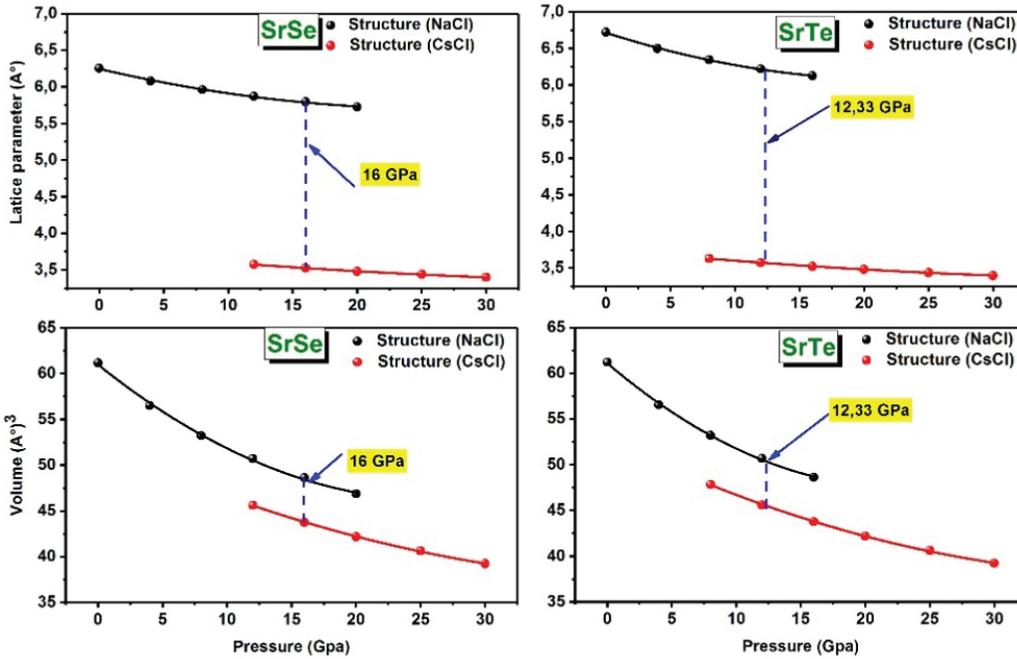


Figure 8. Lattice parameter a and cell volume V as function of the pressure for the SrSe and the SrTe in the two phases. The red line represents the quadratic fit functions of the variation of these parameters with pressure.

Table 4. Quadratic fitting coefficients for the lattice parameters a and cell volume V as functions of the pressure of the two compounds SrSe and SrTe in the two phases B1 and B2

	Phase(B1)			Phase(B2)		
	$x0$	$x1$	$x2$	$x0$	$x1$	$x2$
	$y0$	$y1$	$y2$	$y0$	$y1$	$y2$
SrSe						
a (Å)	6.2459±0.01	-0.0413±0.002	0.00046±1	3.7472±0.007	-0.0165±7.78	0.00016±1
V (Å ³)	60.9926±0.2	-1.1322±0.05	0.0216±0.002	52.3100±0.32	-0.6434±0.03	0.0069±7.65
SrTe						
a (Å)	6.7144±0.009	-0.0567±0.002	0.0012±1.61	3.7575±0.009	-0.0175±5.45	1.8537±1.4
V (Å ³)	61.0880±0.19	-1.1998±0.05	0.0266±0.003	52.8159±0.21	-0.6920±0.02	0.0080±6.48

Table 5. The coefficients of the linear fit polynomial of the relative variation of the lattice and volume parameters, respectively, as functions of the pressure

	Phase B1		Phase B2	
	$X0$	$X1$	$X0$	$X1$
SrSe				
$a/a0$	0.99	-0.004	1.03	-0.002
$V/V0$	0.98	-0.012	1.11	-0.007
SrTe				
$a/a0$	0.99	-0.006	1.03	-0.002
$V/V0$	0.99	-0.014	1.08	-0.007

We see that for the SrSe, the gap’s nature is still indirect. On the other hand, when pressure increases, the SrTe compound’s gap grows indirect. Other cubic structures, such as binary CaX compounds (where X = S, Se, or Te), have also shown this behavior [31–32].

We looked at the gap energies at the selected high symmetry sites as a function of pressure in order to investigate the impact of pressure on the gap energy and the location of the conduction band minimum of the compounds SrSe and SrTe. The relationship between the gap energy and each compound’s hydrostatic pressure during the two stages is shown in Figure 11. The graphs demonstrate how, for both compounds in the two phases,

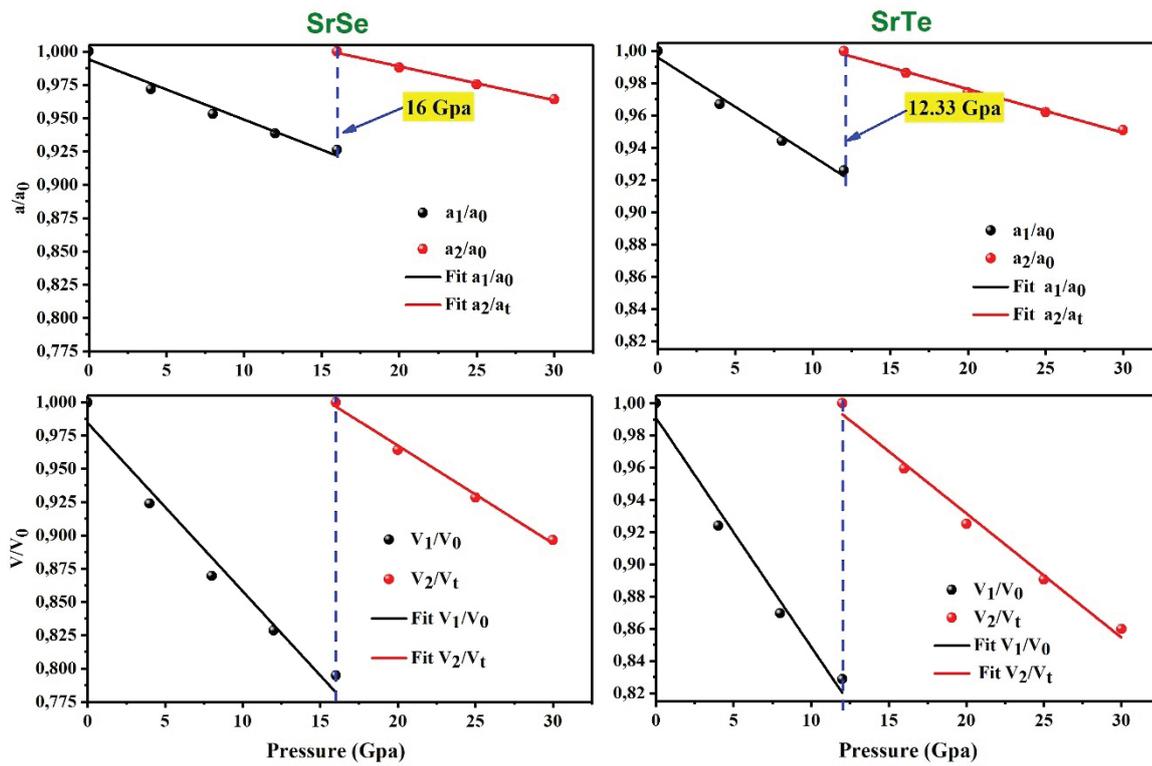


Figure 9. Fitting of the relative variation of the lattice and volume parameters as functions of the pressure for SrSe and SrTe.

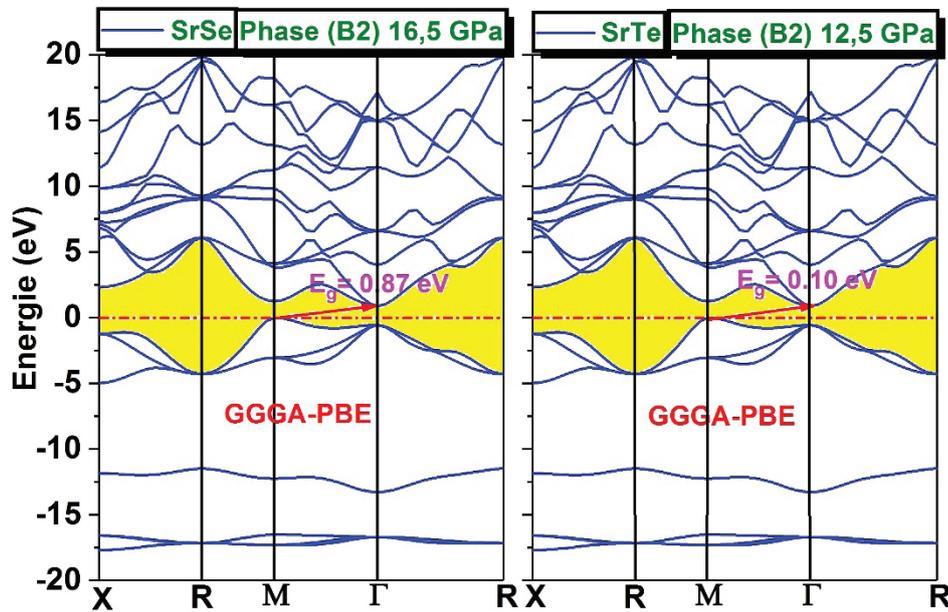


Figure 10. Band structure of SrSe and SrTe at pressures 16.5 GPa and 12.5 GPa.

the gap value falls as hydrostatic pressure increases. To parameterize the function which gives the variation of the gap E_g with the pressure, we consider the following quadratic form:

$$E_g(P) = a + b \cdot P + c \cdot P^2 \tag{3}$$

The parameters of the quadratic fit of the function a , b , and c are given in Table 6. At the phase change point the gap

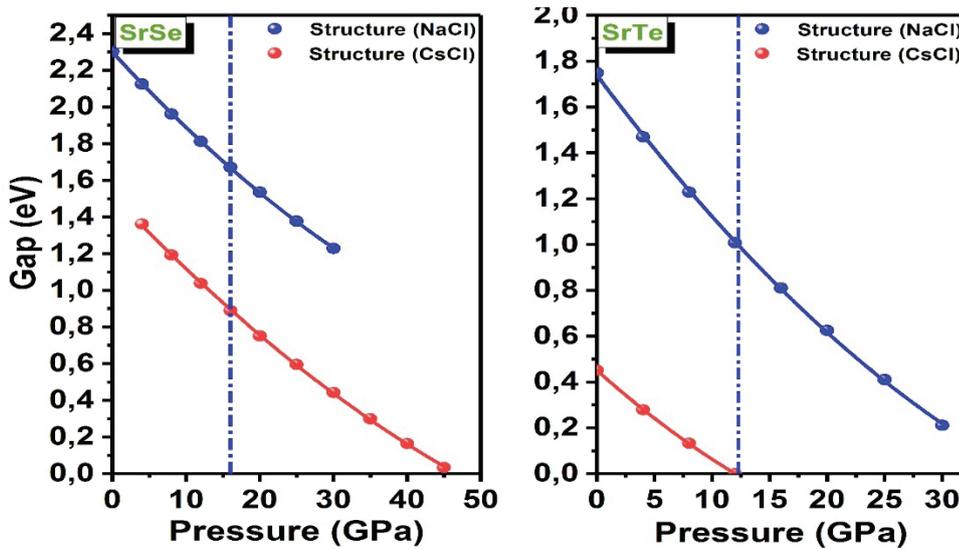


Figure 11. Evolution of the gap energy as function of pressure for SrSe and SrTe.

Table 6. Quadratic fitting coefficients for the gap energy as function of pressure for SrSe and SrTe in phases B1 and B2

	Phase(B1)			Phase(B2)		
	A	b	C	A	B	c
SrSe	2,290± 0,003	-(430,0±5,2) E-4	(27,0±1,6)E-5	1,520± 0,006	-(40,0±6,2)E-4	(21,0±1,2)E-5
SrTe	1,730± 0,008	-(60± 1) E-3	(54,0±4,1)E-5	0,450± 0,002	-0,040± 0,001	(61,0±9,1)E-5

undergoes a sudden variation at 0.78eV for the SrSe and 1eV for the SrTe.

The values of $\Delta E_g = E_g - E_{g_0}$, with E_{g_0} denoting the energy gap at zero pressure, are of the order of 1eV which is a notable change. This result is very important in practice, since a value of 1eV is easily detectable by experiment. As a result, a novel approach to computing the phase transition pressure based on the measurement of gap energy fluctuation may be proposed.

Metallization Effect

From the gap energy evolution as function of the pressure for SrSe and SrTe compounds in phase B2 (Fig. 12), the band structures of the two compounds, SrSe and SrTe, have been displayed at pressures of 64 and 13 GPa, respectively. (Fig. 12). Since the valence band and the conduction band overlap (the gap energy eventually drops to 0 eV), it is evident from the two band structures that the two compounds acquire a metallic nature.

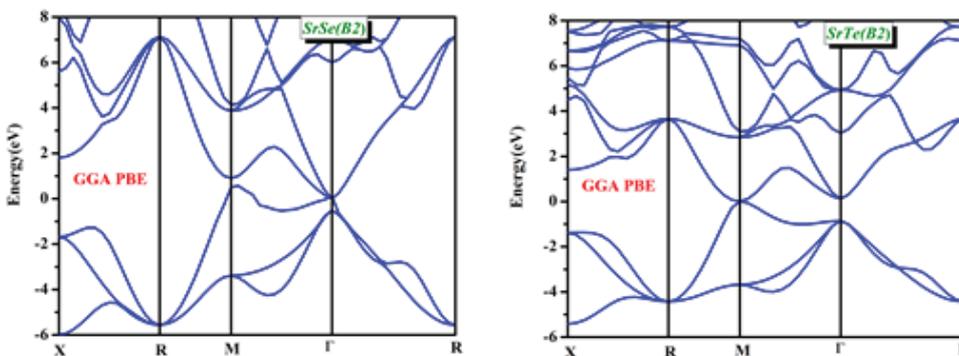


Figure 12. Band structure of SrSe and SrTe at metallic pressures 46 GPa and 13 GPa respective.

Table 7. Metallization pressure P_m (GPa) for SrSe and SrTe compared with other theoretical results

P_m (GPa)	SrSe	SrTe
Our results	46	13
Cal	24 ⁽¹⁾	18 ⁽¹⁾
	48.91 ⁽³⁾	18.17 ⁽³⁾
	-	55 ⁽¹⁾
Exp	>45 ⁽²⁾	-

⁽¹⁾Ref[25]; ⁽²⁾Ref[33]; ⁽³⁾Ref[20]

In this case the two semiconductor materials become metals. The pressure that corresponds to this change is called metallization pressure. Table 7 is a list of the metallization pressure values that were computed in this work. Our model of the heavy alkaline earth chalcogenides is compared to previous existing theoretical and empirical models. We have reasonable agreement between our values for the metallization pressure.

CONCLUSIONS

In this study, we investigated theoretically how pressure affects the structural and electrical characteristics of semiconductors from the SrSe and SrTe family of strontium chalcogenides. The DFT approach, together with the generalized gradient approximation (GGA) and the pseudo-potential and plane wave method (PP_PW), have been used to conduct the computations. The simulations had been implemented with the CASTEP code.

We find good agreement between the experimental data reported in the literature and our estimated lattice parameters of the cubic structure a and the volume V in the two phases B1 (NaCl) and B2 (CsCl) of the two compounds. We discovered that these compounds experience phase transitions at hydrostatic pressure of around 16 GPa for SrSe and 12.33 GPa for SrTe. An indirect gap exists in the Γ -X direction, according to analysis of the band structure at zero pressure. We investigated how pressure affected the two compounds' physical characteristics throughout phases B1 and B2. The obtained results unambiguously demonstrate that, in contrast to the gap's nearly linear reduction with pressure, the lattice parameter fluctuates quadratically. Additionally, we have discovered that the SrTe compound gap becomes direct, but the SrSe gap remains indirect. Phase B2 turns metallic (zero gap) at pressures over 46 GPa for SrSe and 13 GPa for SrTe. Our results have greater credibility since they are in good accord with several theoretical and experimental works, as demonstrated by the results reported in this study.

ACKNOWLEDGMENTS

The authors are grateful to Pr A. El Hdiy (ITheMM/EA7548), Université de Reims Champagne-Ardenne,

Reims, France) and Dr O. Houhou (Laboratory of Physics of Experimental Techniques and Applications, University of Medea, Medea 26000, Algeria) for valuable discussions. This work was supported by the Algerian ministry of higher education and scientific (MESRS) and The General Directorate of Scientific Research and Technological Development (DGRSDT).

AUTHORSHIP CONTRIBUTIONS

Authors equally contributed to this work.

DATA AVAILABILITY STATEMENT

The authors confirm that the data that supports the findings of this study are available within the article. Raw data that support the finding of this study are available from the corresponding author, upon reasonable request.

CONFLICT OF INTEREST

The author declared no potential conflicts of interest with respect to the research, authorship, and/or publication of this article.

ETHICS

There are no ethical issues with the publication of this manuscript.

REFERENCES

- [1] Han P, Bester G. Force field potentials for the vibrational properties of II-VI semiconductor nanostructures. *Physical Rev B* 2017;96:195436. [\[CrossRef\]](#)
- [2] Chandra BP, Chandra VK, Jha P. Luminescence of II-VI semiconductor nanoparticles. *Solid State Phenom* 2015;22:1–65. [\[CrossRef\]](#)
- [3] Salam MMA. First principles study of structural, elastic and electronic structural properties of strontium chalcogenides. *Chin J Phys* 2019;57:418–434.
- [4] Bhattacharjee R, Chattopadhyaya S. Effects of doping of calcium atom(s) on structural, electronic and optical properties of binary strontium chalcogenides - A theoretical investigation using DFT based FP-LAPW methodology. *Solid State Sci* 2017;71:92–110. [\[CrossRef\]](#)
- [5] Chattopadhyaya S, Bhattacharjee R. DFT based FP-LAPW investigation of structural, electronic and optical properties of $Sr_xPb_{1-x}S$, $Sr_xPb_{1-x}Se$ and $Sr_xPb_{1-x}Te$ ternary alloys. *J Alloys Compd* 2017;698:868–882. [\[CrossRef\]](#)
- [6] Asano S, Yamashita N, Ogawa Y. Luminescence et structure vibrationnelle des luminophores $CaS:Ce^{3+}$ et $CaSe:Ce^{3+}$. *Phys Stat Solid* 1983;118:89–100. [\[CrossRef\]](#)

- [7] Yamaoka S, Shimomura O, Nakazawa H, Fukunaga O. Pressure-induced phase transformation in BaS. *Solid State Commun* 1980;33:87–89. [\[CrossRef\]](#)
- [8] Baby T, Nampoori V. Fluorescence emission of SrS: Eu²⁺ phosphor-energy level splitting of Eu²⁺. *Solid State Commun* 1992;81:367–369. [\[CrossRef\]](#)
- [9] Zimmer, Winzen H, Syassen K. High-pressure phase transitions in CaTe and SrTe. *Physical Rev B* 1985;32:4066. [\[CrossRef\]](#)
- [10] Luo H, Greene RG, Ruoff AL. High-pressure phase transformation and the equation of state of SrSe. *Physical Rev B* 1994;49:15341. [\[CrossRef\]](#)
- [11] Kaneko Y, Koda T. New developments in IIA-VIb (alkaline-earth chalcogenide) binary semiconductors. *J Crystal Growth* 1988;86:72–78. [\[CrossRef\]](#)
- [12] Jha PK, Sakalle UK, Sanyal SP. High pressure structural phase transition in alkaline earth chalcogenides. *J Phys Chem Solids* 1998;59:1633–1637. [\[CrossRef\]](#)
- [13] Rajput K, Roy DR. Structure, stability, electronic and thermoelectric properties of strontium chalcogenides. *Physica E Low Dimens Syst Nanostruct* 2020;119:113965. [\[CrossRef\]](#)
- [14] Debnath B, Sarkar U, Debarma M, Bhattacharjee R, Chattopadhyaya S. Tuning of electronic band gaps and optoelectronic properties of binary strontium chalcogenides by means of doping of magnesium atom(s)- a first principles based theoretical initiative with mBJ, B3LYP and WC-GGA functionals. *Phys B Phys Condens Matter* 2018;530:53–68. [\[CrossRef\]](#)
- [15] Rahman S, Saqib H, Liang X, Errandonea D, Resta AS, Molina-Sanchez A, et al. Pressure-induced metallization and robust superconductivity in pristine 1T-HfSe₂. *Mater Today Phys* 2022;25:100698. [\[CrossRef\]](#)
- [16] Segall MD, Lindan PJD, Probert MJ, Pickard CJ, Hasnip PJ, Clark SJ, et al. First-principles simulation: ideas, illustrations and the CASTEP code. *J Phys Condens Matter* 2002;14:2717. [\[CrossRef\]](#)
- [17] Kohn W, Sham LJ. Self-consistent equations including exchange and correlation effects. *Phys Rev* 1965;140:A1133–A1138. [\[CrossRef\]](#)
- [18] Perdew JP, Burke K, Ernzerhof M. Generalized gradient approximation made simple. *Phys Rev Lett* 1996;77:3865. [\[CrossRef\]](#)
- [19] Vanderbilt D. Soft self-consistent pseudopotentials in a generalized eigenvalue formalism. *Physical Rev B* 1990;41:7892–7895. [\[CrossRef\]](#)
- [20] Yang X, Ai-Min H, Jie Y, Yong-Hao H, Gang P, Chun-Xiao G, et al. Theoretical prediction for structural stabilities and optical Properties of SrS, SrSe and SrTe under high pressure. *Phys Lett* 2008;25:1807. [\[CrossRef\]](#)
- [21] Bouchenafa M, Benmakhlouf A, Sidoumou M, Bouhemadou A, Maabed S, Halit M, et al. Theoretical investigation of the structural, elastic, electronic, and optical properties of the ternary tetragonal tellurides KBTe₂ (B = Al, In). *Mater Sci Semiconductor Proces* 2020;114:105085. [\[CrossRef\]](#)
- [22] Khenata R, Baltache H, Rivat M, Driz M, Sahnoun M, Bouhafs B, et al. First-principle study of structural, electronic and elastic properties of SrS, SrSe and SrTe under pressure. *Phys B Condens Matter* 2003;339:208–215. [\[CrossRef\]](#)
- [23] Souadkia M, Bennecer B, Kalarasse F, Mellouki A. Ab initio calculation of vibrational and thermodynamic properties of SrX (S, Se, Te) in the B1 (NaCl) and B2 (CsCl) structures. *Comput Mater Sci* 2011;50:1701–1710. [\[CrossRef\]](#)
- [24] Lany S, Zunger A. Polaronic hole localization and multiple hole binding of acceptors in oxide wide-gap semiconductors. *Phys Rev B* 2009;80:085202. [\[CrossRef\]](#)
- [25] Shameem Banu IB, Rajagopalan M, Palanivel B, Kalpana G, Shenbagaraman P. Structural and electronic properties of SrS, SrSe, and SrTe under pressure. *Journal of Low Temperature Physics* 1998;112:211–226. [\[CrossRef\]](#)
- [26] Lines ME. Bond-orbital theory of linear and non-linear electronic response in ionic crystals. I. Linear response. *Phys Rev B* 1990;41:3383–3390. [\[CrossRef\]](#)
- [27] Syassen K, Christensen N, Winzen H, Fischer K, Evers J. Optical response and band-structure calculations of alkaline-earth tellurides under pressure. *Phys Rev B* 1987;35:4052. [\[CrossRef\]](#)
- [28] Shi L, Duan Y, Yang X, Qin L. Structural phase transition, electronic and elastic properties of SrSe under pressure from first-principles calculations. *Comput Mater Sci* 2010;49:524–529. [\[CrossRef\]](#)
- [29] Labidi S, Meradji H, Labidi M, Ghemid S, Drablia S, El Haj Hassan F. First principles calculations of structural, electronic and thermodynamic properties of SrS, SrSe, SrTe compounds and SrS_{1-x}Se_x alloy. *Phys Proced* 2009;2:1205–1212. [\[CrossRef\]](#)
- [30] Bahloul B, Bentabet A, Amirouche L, Bouhadda Y, Bounab S, Deghfel B, et al. Ab initio calculations of structural, electronic, optical and thermodynamic properties of alkaline earth tellurides BaSr_{1-x}Te. *J Phys Chem Solids* 2014;75:307–314. [\[CrossRef\]](#)
- [31] Charifi Z, Baaziz H, El Haj Hassan F, Bouarissa N. High pressure study of structural and electronic properties of calcium chalcogenides. *J Phys Condens Matter* 2005;17:4083–4092. [\[CrossRef\]](#)
- [32] Hao JH, Wu ZQ, Wang Z, Jin QH, Li BH, Ding DT. First principles calculations of structural phase transformation in CaTe at high pressure. *Physica B Condens Matter* 2009;404:3671–3673. [\[CrossRef\]](#)
- [33] Atkinson TD, Chynoweth KM, Cervantes P. Electronic band gap of SrSe at high pressure. *Solid State Commun* 2006;139:215–217. [\[CrossRef\]](#)