

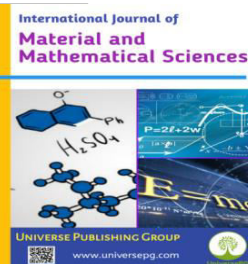


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The Physical Properties of ThCr_2Si_2 - Type Co-based Compound SrCo_2Si_2 : An *ab-initio* Study

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ABSTRACT

In this article, we have studied the mechanical, electronic, and optical features of ThCr_2Si_2 - type compound SrCo_2Si_2 . The investigation has been done by using the first-principles method depend on the density functional theory (DFT) and the calculations were completed with the Cambridge Serial Total Energy Package (CASTEP) code. The optimized lattice parameters are well in accord with the existing synthesized values. The investigated elastic constants for this compound are positive which ensured the mechanical stability of this phase. The calculated values of Pugh's ratio and Poisson's ratio ensure the brittle character of SrCo_2Si_2 . The universal anisotropic constant A^U ensures the anisotropic behavior of SrCo_2Si_2 . The softness nature of SrCo_2Si_2 is confirmed by the bulk modulus calculations. The overlapping of the valence band and conduction band near the Fermi level indicates the metallic nature of SrCo_2Si_2 . At the Fermi level the major contribution comes from Co-3d and Si-3p states. The large reflectivity in the high-energy region indicates that this compound might be useful as coating materials for reducing solar heating. The photoconductivity and absorption begin with zero photon energy which also ensures the metallic nature of SrCo_2Si_2 .

Keywords: Co-based compound SrCo_2Si_2 , Structural properties, Electronic properties, and Optical properties.

1. INTRODUCTION:

ThCr_2Si_2 type ternary intermetallic materials usually hold a superconducting ground position. The rare-earth AM_2X_2 structural materials have received great interest of researchers because of their many rich characteristics. Recently AM_2X_2 (where, A is a lanthanide element or any alkaline earth element; M is any transition metal; X = P, Ge, Si or As) type compounds have achieved great interest having their many interesting features such as mixed valency, superconductivity at both high and low temperature, valence fluctuation and heavy fermions behavior (Stewart, 2001). These types of transition metal with AM_2X_2 type structure confirm extremely good-looking and wealthy physics in view of the fact that of their close energies relating to the spin, charge

and orbital motion (Imada *et al.*, 1998). There are more than two thousand classes of ternary intermetallic compounds (Villars and Genzual, 2007) which are essentially obtained from the BaAl_4 type structures. Among these classes ThCr_2Si_2 type compounds were first discovered and illustrated in 1965 by Ban and Sikirica, (1965). A complete and acceptable geometric assessment of about six hundred phases of ThCr_2Si_2 - type structures are represented by Just and Pauffer, (1996).

In recent times ThCr_2Si_2 - type structure has gained massive consideration of researchers after discovering a new superconductor ($\text{Ba}_{0.6}\text{K}_{0.4}$) Fe_2As_2 belongs to the "122" family of iron-arsenide's with ThCr_2Si_2 type structure exhibits high transition tem-

perature 38K (Rotter *et al.*, 2008). On the other hand, Pt, Ni and Pd-based ThCr_2Si_2 type borocarbides (Nagarajan *et al.*, 1994; Cava *et al.*, 1994; Batlogg *et al.*, 1994) have been discovered in the recent years with the transition temperature up to 23K which raises the hope to constitute a family of new high temperature superconductors. In iron-based compounds, the ternary intermetallic (122-type compounds) in the company of ThCr_2Si_2 type structure as example AFe_2As_2 (A = Sr, Ca, Ba, etc.) are free from oxygen having metallic nature (Rotter *et al.*, 2008; Sasmal *et al.*, 2008; Torikachvili *et al.*, 2008). These types of compounds have been comprehensively studied for interpreting their superconducting mechanism (Johnston 2010; Stewart 2011). These types of compounds have high chemical flexibility and abundance of substitution possibilities. In recent times concentration was given to a series of the iron based and arsenic-free AeT_2X_2 compounds (Ae = alkaline earth metal, T = Ni, Pd; X = P, Ge) with very low transition temperatures ($T_c \sim 0.3 - 3.0$ K) (Mine *et al.*, 2008). Undoped RT_2Si_2 (R = La, Y, Th; T = Ir, Pt) type superconductors are predicted to CaBe_2Ge_2 -type structures (Yang *et al.*, 2011). However the compounds with alkaline earth metals having ThCr_2Si_2 - type structure are inadequate (Ronning *et al.*, 2009; Fujii and Sato, 2009; Shelton *et al.*, 1984; Doerrscheidt *et al.*, 1976; Rieger and Parthé, 1969; Bodak and Gladyshevskii, 1968; Palenzona *et al.*, 1987).

In this work we have studied a new phase with alkaline earth metal on the A-site crystallizing in the ThCr_2Si_2 - type structure are inadequate. The compound SrCo_2Si_2 signifies the third ternary SrT_2Si_2 compound (T = 3d-block transition metals) besides SrCu_2Si_2 (Kranenberg *et al.*, 2002) and SrZn_2Si_2 (May and Schäfer, 1972). For SrT_2Si_2 the isostructural compounds with T = Pd, Ag have been characterized and reported (Eisenmann *et al.*, 1970). The compound SrCo_2Si_2 is isoelectronic to the parent Fe-pnictide superconductors AeFe_2As_2 at the X site, contrast to their electronic bonding situation will be of special interest. Here we have studied the detailed physical properties of Co-based material SrCo_2Si_2 by using the DFT based calculations implemented in CASTEP code.

2. Computational details

The CASTEP code (Segall *et al.*, 2002) written by FORTRAN 95 language is used to investigate the physical properties of SrCo_2Si_2 . The calculations UniversePG | www.universepg.com

were done by DFT theory within GGA with the PBE exchange-correlation function (Clark *et al.*, 2005; Materials Studio CASTEP, 2010; Hohenberg and Khon, 1964; Perdew *et al.*, 2008). The pseudo atomic calculations were done for Sr-4s² 4p⁶ 5s², Si-3s² 3p² and Co-3d⁷ 4s² valence electrons. The plane wave cut-off energy was set to 500 eV. The special k-point sampling of the Brillouin zone (BZ) was employed by using the Monkhorst-Pack method (Monkhorst and Pack, 1976) with special 10×10×10 grid points in the primitive cell of SrCo_2Si_2 . The crystal structure of SrCo_2Si_2 was optimized by the Broyden-Fletcher-Goldfarb-Shanno (BFGS) minimization technique (Pfrommer *et al.*, 1997). For this optimization the criteria of convergence were set to 1.0×10^{-5} eV/atom for energy, 0.03 eV/Å for force, 0.05 Gpa for stress and 0.001 Å for ionic displacement. The elastic stiffness constants of SrCo_2Si_2 were obtained by the stress-strain method (Fan *et al.*, 2006). Then the bulk properties were obtained by the elastic constant data of SrCo_2Si_2 . In that case the criteria of convergence tolerance were set to 2.0×10^{-6} eV/atom for energy, 2.0×10^{-4} Å for maximum ionic displacement, 6.0×10^{-3} eV/Å for maximum ionic force and 0.1 GPA for maximum stress component. The maximum strain amplitude was set to be 0.003 in the present calculation of SrCo_2Si_2 .

3. RESULT AND DISCUSSION:

3.1 Structural properties - At normal temperature and pressure, SrCo_2Si_2 possesses a tetragonal crystal structure with the space group of I4/mmm (no.139) (Hoffmann *et al.*, 2012). The conventional and optimized crystal structures of SrCo_2Si_2 are shown in **Fig 1**. The unit cell contains two formula units (Z=2) with ten atoms that means one formula unit for each primitive cell with five atoms. The atomic position of Sr, Co, and Si in the unit cell of SrCo_2Si_2 tetragonal crystal are 2a (0 0 0), 4d (0 0.5, 0.25) and 4e (0 0 0.3606) respectively.

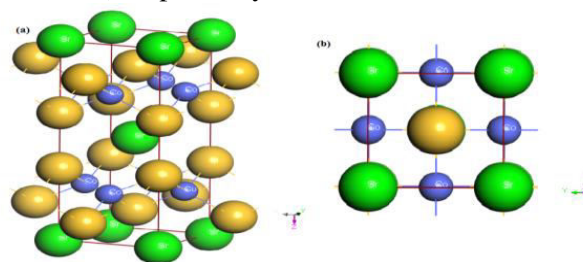


Fig 1: The crystal structures of SrCo_2Si_2 (a) Conventional unit cell (three dimensional); (b) Primitive cell (two dimensional).

Table 1: The calculated equilibrium lattice parameters, unit cell volume, bulk modulus of ThCr₂Si₂-type SrCo₂Si₂ compound in comparison with available experimental data.

Properties	SrCo ₂ Si ₂		Deviation from Expt. (%)
	This work	Experimental	
a_0 (Å)	3.939	3.974	0.8807
c_0 (Å)	10.601	10.395	1.982
c_0/a_0	2.668	2.616	1.988
V_0 (Å ³)	166.9	164.2	1.644
B_0 (Gpa)	75.73	80.6	6.042

The unit cell dimensions including equilibrium lattice parameters for tetragonal phase a_0 and c_0 , bulk modulus B_0 and the equilibrium cell volume V_0 of SrCo₂Si₂ intermetallics at ambient temperature are charted in **Table 1** with the experimentally evaluated values. From **Table 1** it is obvious that the calculated lattice parameters are exceedingly close to the experimental data which ensure the dependability of the DFT- based investigations. From **Table 1** we have seen that, our calculated lattice parameters are slightly deviated from the experimental results. The motive is due to the temperature dependence of the lattice parameters and GGA route (Zhu *et al.*, 2016).

3.2 Elastic properties - Elastic constants are very vital parameters which help us by providing the information about the nature of force present in a solid material. A proper explanation about the mechanical and dynamical behavior of crystalline solid is provided by the analysis of elastic constants. These properties also ensure the mechanical stability, rigidity

and ductile/brittle nature of a solid material (Gole-sorkhtabar *et al.*, 2013; Koç *et al.*, 2012). Different important properties of solid materials such as ductility, anisotropy, stiffness, brittleness and stability can be derived from the elastic constant data (Rahaman *et al.*, 2016). Hence in this article a thorough investigation into the mechanical nature of SrCo₂Si₂ has been done with accurate discussion and composition. The elastic constants were achieved from a linear fit of the calculated stress-strain function according to Hook’s law (Nye, 1961). A crystal with the tetragonal phase belongs to six independent elastic constants (C_{11} , C_{12} , C_{13} , C_{33} , C_{44} and C_{66}).The estimated elastic constants of SrCo₂Si₂ are listed in **Table 2**. According to the stability criteria (Pokunov *et al.*, 2004) of tetragonal phase (Eq. 1) the compounds under consideration have good stability in nature.

$$\begin{aligned}
 &C_{11} > 0, C_{33} > 0, C_{66} > 0, C_{44} > 0 \\
 &C_{11} + C_{33} - 2C_{13} > 0, C_{11} - C_{12} > 0 \\
 &2(C_{11} + C_{12}) + 4C_{13} + C_{33} > 0
 \end{aligned} \tag{1}$$

Table 2: The evaluated elastic constants C_{ij} (in GPa) of SrCo₂Si₂ with similar type of compounds

Compounds	C_{11}	C_{12}	C_{13}	C_{33}	C_{44}	C_{66}	Ref.
SrCo ₂ Si ₂	196.72	54.35	45.13	92.79	69.66	83.77	This work
SrRu ₂ As ₂	181.95	57.08	48.31	120.74	49.23	70.40	Chowdhury <i>et al.</i> , 2019
SrRh ₂ Ge ₂	179.5	72.4	52.2	103.6	52.6	80.9	Salma <i>et al.</i> , 2018

By utilizing the evaluated data of C_{ij} , the most important mechanical features such as bulk modulus B , shear modulus G , Young’s modulus Y , anisotropy factor A and Poisson’s ratio ν of intermetallic SrCo₂Si₂ have been calculated by using the Voigt-Reuss-Hill (VRH) averaging scheme (Hill, 1952). Which are listed in **Table 3**. The Voigt and Reuss bounds of B and G for cubic systems can be represented by the following expressions.

$$B_v = \frac{2C_{11} + 2C_{12} + C_{33} + 4C_{13}}{9} \tag{2}$$

$$B_R = C^2 / M \tag{3}$$

$$G_v = M + 3C_{11} - 3C_{12} + 12C_{44} + 6C_{66} / 30 \tag{4}$$

$$G_R = \frac{15}{\left[\frac{18B_v}{C^2} + \frac{6}{(C_{11} - C_{12})} + \frac{6}{C_{44}} + \frac{3}{C_{66}} \right]} \tag{5}$$

Where, M and C^2 can be written as,

$$M = C_{11} + C_{12} + 2C_{33} - 4C_{13} \text{ and } C^2 = (C_{11} + C_{12}) C_{33} - 2C_{13}^2$$

The arithmetic mean value of the Voigt (B_v , G_v) and the Reuss (B_R , G_R) bounds which is used to calculate the polycrystalline modulus is given by in terms of Voigt-Reuss-Hill approximations:

$$B_H = B = \frac{1}{2}(B_R + B_v) \tag{6}$$

$$G_H = G = \frac{1}{2}(G_v + G_R) \quad (7)$$

Using the following expressions we have also calculated the Young's modulus (Y) and Poisson's ratio (ν),

$$Y = \frac{9GB}{3B + G} \quad (8)$$

$$\nu = \frac{3B - 2G}{2(3B + G)} \quad (9)$$

The Young's modulus is specified by the ratio of the tensile stress to tensile strain, which measure the stiffness for solid material. The larger value of Y point outs the more stiffness of a compound (Chen, *et al.*, 2011). The higher value makes the solid better stiffer. The calculated Young's modulus is shown in **Table 3** along with available similar type of compounds. From **Table 3**, we can say that the value of Young's modulus of $SrCo_2Si_2$ is larger than $SrRu_2As_2$ and $SrRh_2Ge_2$ compounds indicating that

the compound $SrCo_2Si_2$ is stiffer than $SrRu_2As_2$ and $SrRh_2Ge_2$ compounds.

The Poisson's ratio is another useful parameter to understand the nature of bonding force in a material (Cao *et al.*, 2013). The smaller value of ν ($\nu = 0.1$) indicates the covalent materials whereas for ionic crystal $\nu = 0.25$. The larger value of Poisson's ratio ($\nu > 0.26$) indicates that the compound will be ductile and the compound will be brittle when the value of Poisson's ratio is ($\nu < 0.26$). From **Table 3**, we see that the value of ν is 0.18 which refers the brittle nature of $SrCo_2Si_2$. The ratio between bulk and shear modulus (B/G) is known as Pugh's ratio which is applied to understand the brittleness and ductility manner of solid material (Pugh, 1954). According to Pugh's criteria a material should be brittle if it's $B/G < 1.75$, otherwise it should be ductile. From our calculations we see that $B/G < 1.75$, hence the material $SrCo_2Si_2$ shows brittle manner which is very similar to Poisson's ratio.

Table 3: Evaluated polycrystalline bulk modulus B (GPa), shear modulus G (GPa), Young's modulus E (GPa), B/G value, Poisson's ratio ν and elastic anisotropy A^U of $SrCo_2Si_2$ with similar types of compounds.

Compounds	B	G	Y	B/G	ν	A^U	Ref.
$SrCo_2Si_2$	80.60	64.44	152.64	1.25	0.18	0.629	This work
$SrRu_2As_2$	86.11	55.03	136.05	1.56	0.23	0.180	Chowdhury <i>et al.</i> , 2019
$SrRh_2Ge_2$	86.60	54.40	134.70	1.59	0.24	0.469	Salma <i>et al.</i> , 2018

The universal anisotropic factor of a solid material is specified by the subsequent relation (Ranganathan, *et al.*, 2008).

$$A^U = \frac{5G_v}{G_R} + \frac{B_v}{B_R} - 6 \quad (10)$$

$A^U = 0$ indicates completely isotropic crystal and the deviation from this value shows the degree of anisotropy in a material. Chung and Buessem suggests two new relations (Chung and Buessem, 1967) to determine the anisotropy indexes of bulk modulus and shear modulus given as follows,

$$A_B = \frac{(B_v - B_R)}{(B_v + B_R)} \quad (11)$$

$$A_G = \frac{(G_v - G_R)}{(G_v + G_R)} \quad (12)$$

For an isotropic crystal the value of A is 1 and for anisotropic crystal the values of A are either smaller or greater than unity. From **Table 3** we see that the value of A is less than unity which represents the anisotropic nature of this compound.

3.3 Electronic properties - The band structure and density of states (TDOS and PDOS) provide a clear concept about the electronic properties of a material. The electronic band structure provides vital information about a material to be metal, semiconductor or insulator. The bonding features of a material are obtained from the partial and total density of states calculations (Hu, *et al.*, 2014). The full picture of energy bands and band gaps of a solid is known as electronic band structure or simply band structure. In solid-state and condensed matter physics, the band structure defines certain ranges of energy that are allowed for electrons within a solid, and the ranges of energy that are not allowed for any electrons. The investigated band structure for $SrCo_2Si_2$ has been illustrated in **Fig 2** in the energy range -10 eV to 10 eV which is observed along the high symmetry directions in the first Brillouin zone. The horizontal solid line at 0 eV indicates the Fermi level. From band structure it has seen that the valence bands and conduction bands are overlapped at Fermi level and there is no band gap indicating that this compound

shows metallic manner. The metallic nature of SrCo₂Si₂ signifies that this compound might be superconductor. The partial and total density of states of SrCo₂Si₂ is plotted in **Fig 3**. From **Fig 3** we have observed that the total density of states (TDOS) of SrCo₂Si₂ is composed of four main peaks.

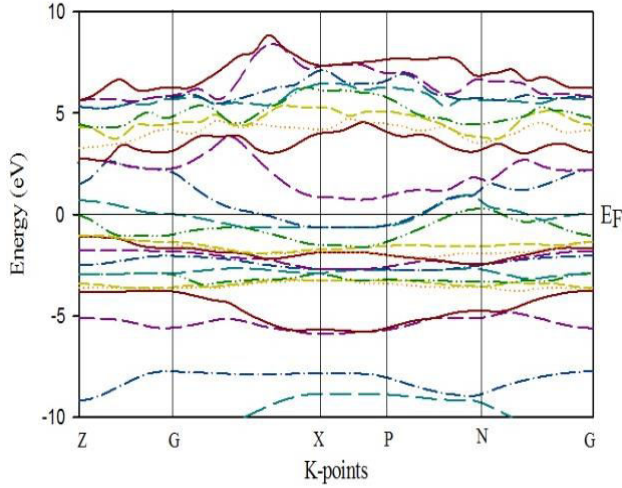


Fig 2: The band structure of compound SrCo₂Si₂.

The first peak in the valence band lies between -36.17 eV and -34.75 eV. In SrCo₂Si₂, Sr-5s states contribute the most to create the first peak. The second peak lies between -18.63 eV and -16.93 eV in SrCo₂Si₂. This peak is dominated by Co-3d and Si-3p states. The third peak lies between -11.42 eV and -7.46 eV. This peak is contributed by Si-3p states. The fourth peak lies from -6.32 eV to 8.65 eV. This peak is dominated by Si-3s and Si-3p states. We observe clear coincidence between the Co-3d and Si-3p states in SrCo₂Si₂, which suggests the covalent nature of Co-Si bonds in SrCo₂Si₂ (Rahman *et al.*, 2016). This is a common feature of ThCr₂Si₂ type compounds (Jeitschko *et al.*, 1987). The calculated DOS at EF is 3.43 states/ eV-unit cell.

3.4 Optical properties - The study of photon energy dependent optical function of a solid material is so essential due to the fact that it helps to get a clear conception concerning the electronic configuration of materials. The optical properties of SrCo₂Si₂ with different photon energies are calculated by the frequency dependent dielectric function, $\epsilon(\omega) = \epsilon_1(\omega) + i\epsilon_2(\omega)$, which is closely correlated to the electronic configurations. The imaginary part $\epsilon_2(\omega)$ of dielectric function is obtained from the momentum matrix elements between the filled and the unfilled electronic state by utilizing the subsequent relation (Materials Studio CASTEP, 2010);

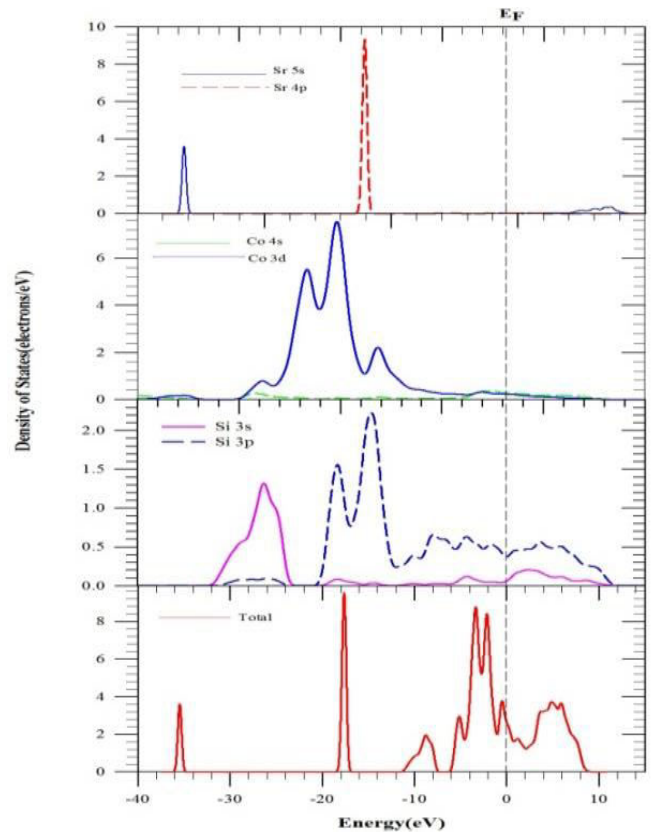


Fig 3: The calculated density of states (TDOS and PDOS) of SrCo₂Si₂.

$$\epsilon_2(\omega) = \frac{2e^2\pi}{\Omega\epsilon_0} \sum_{k,v,c} \left| \langle \psi_k^c | \hat{u} \cdot \vec{r} | \psi_k^v \rangle \right|^2 \delta(E_k^c - E_k^v - E) \quad (13)$$

Where, ω refers to light frequency, e indicates the electronic charge, \hat{u} is the vector representing the polarization of the incident electric field, along with ψ_k^c and ψ_k^v are the conduction band and valence band wave functions at k , successively. From the imaginary part $\epsilon_2(\omega)$, the real part $\epsilon_1(\omega)$ of the dielectric function is obtained through the Kramers-Kronig relations.

$$\epsilon_1(\omega) = 1 + \frac{2}{\pi} P \int_0^\infty \frac{\omega' \epsilon_2(\omega')}{\omega'^2 - \omega^2} d\omega' \quad (14)$$

Where, ω denotes the light frequency and P refers the principle value of the integral part.

The reflectivity spectra are derived from Fresnel's formula for normal incidence assuming an orientation of the crystal surface parallel to the optical axis using the relation (Fox, 2001).

$$R(\omega) = \left| \frac{\sqrt{\epsilon(\omega)} - 1}{\sqrt{\epsilon(\omega)} + 1} \right|^2 \quad (15)$$

We calculate the absorption coefficient $I(\omega)$, the real part of optical conductivity $\text{Re}[\sigma(\omega)]$ and the elec-

tron energy-loss spectrum $L(\omega)$ using the following expressions (Delin *et al.*, 1996).

$$I(\omega) = \sqrt{2}(\omega) \left(\sqrt{\varepsilon_1(\omega)^2 + \varepsilon_2(\omega)^2} - \varepsilon_1(\omega) \right)^{1/2} \quad (16)$$

$$\text{Re}[\sigma(\omega)] = \frac{\omega \varepsilon_2}{4\pi} \quad (17)$$

$$L(\omega) = \frac{\varepsilon_2(\omega)}{\varepsilon_1(\omega)^2 + \varepsilon_2(\omega)^2} \quad (18)$$

The optical spectra such as the refractive index, $n(\omega)$, and the extinction coefficient, $k(\omega)$, are easily calculated in terms of the components of the complex dielectric function as follows:

$$n(\omega) = \left[\frac{\varepsilon_1(\omega)}{2} + \frac{\sqrt{\varepsilon_1(\omega)^2 + \varepsilon_2(\omega)^2}}{2} \right]^{1/2} \quad (19)$$

$$k(\omega) = \left[\frac{\sqrt{\varepsilon_1(\omega)^2 + \varepsilon_2(\omega)^2}}{2} - \frac{\varepsilon_1(\omega)}{2} \right]^{1/2} \quad (20)$$

The photon energy dependent ground state optical properties of SrCo₂Si₂ are shown in **Fig 4** in the energy range up to 50 eV along the [100] direction. For optical properties investigation we have used a 0.5 eV Gaussain smearing.

3.4.1 Reflectivity - Reflectivity is a surface-sensitive analytical technique used in Physics, Chemistry and material science to characterize surfaces, thin films and multi layers. The optical reflectivity spectra are shown in **Fig 4(a)** as a function of incident photon energy. For SrCo₂Si₂ the reflectivity spectrum starts with a value of 0.48, at the beginning it decreases and then rises again to reach maximum value of 0.79 at 13.22 eV obtained in the high energy region. This high value of reflectivity in high energy region reveals the characteristics of high conductance in the low energy region (Ali *et al.*, 2016). Hence the compound shows promises as good was coating materials in the ultraviolet region.

3.4.2 Absorption Coefficient - The absorption coefficient visualizes how far into a material light of a particular wave length can penetrate before it is absorbed. The absorption coefficient depends on the material and also on the wavelength of light which is being absorbed. The photon energy dependent absorption spectra of SrCo₂Si₂ are shown in **Fig 4(b)**. For this compound the absorption spectra starts at zero photon energy which ensures the metallic manner of this phase. This phase exhibit quite good absorption coefficient in the energy ranges 4-22 eV. It supplies the information about the optimum solar

energy conversion efficiency and point out the penetration depth of light of precise energy into the material before being absorbed (Ali *et al.*, 2016). For this phase the strong absorption coefficients are observed in the UV region, however, they are weak in the visible region but continuously increase to-ward the UV region, and reach a maximum value at 9.11 eV. This result indicates that this compound is promising for absorbing materials in the UV region.

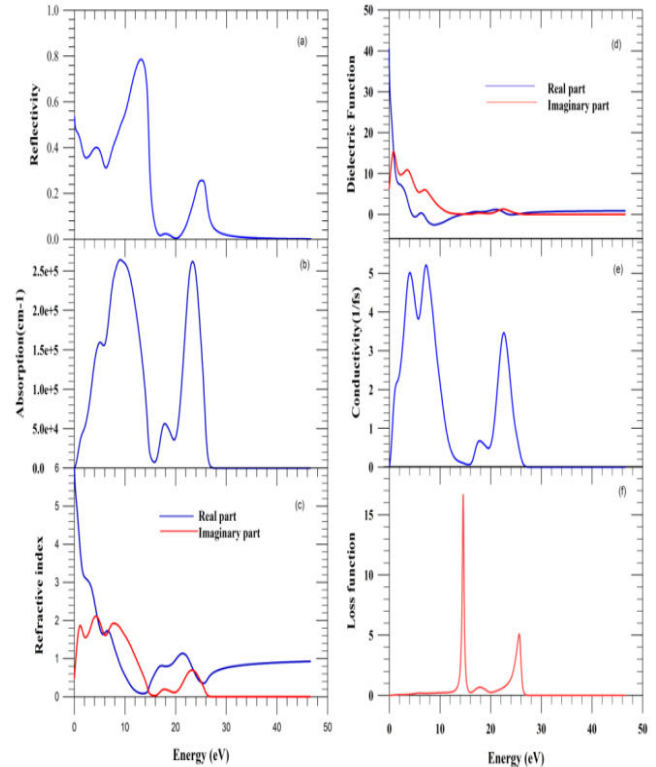


Fig 4: The optical functions: (a) reflectivity, (b) absorption, (c) refractive index, (d) dielectric function, (e) conductivity and (f) loss-function of SrCo₂Si₂ along [100] direction.

3.4.3 Refractive index - Refractive index is a dimensionless quantity which determines how much light is bent or refracted when entering into material (Russell, 2003). The concept of refractive index of optical material is important for use in optical instruments like optical crystals, waveguides etc. **Fig 4(c)** shows the refractive index of SrCo₂Si₂ which is one of the important optical properties. In the low energy region the highest refractive index of SrCo₂Si₂ was found to 6.0 and this value rapidly decreases in the high energy region.

3.4.4 Dielectric function - An important optical function of solid material is the dielectric function which illustrates how an element responds to an electromagnetic wave. The dielectric function of a material describes the electrical and optical properties versus

frequency, wavelength, or energy. It describes the polarization (electric polarizability) and absorption properties of the material. **Fig 4(d)** shows the real $\epsilon_1(\omega)$ and imaginary $\epsilon_2(\omega)$ part of dielectric function of SrCo₂Si₂. The static value of dielectric constant is 40.80. The real part $\epsilon_1(\omega)$ goes to below from zero and back to zero up to 46.72 eV. The imaginary part for compound SrCo₂Si₂ starts from 6.04 and highest peak is 15.84 at 0.72 eV and decrease continuously to zero up to 46.72 eV. The value of 46.72 eV indicating the limit of dielectric function of SrCo₂Si₂, above this value the material becomes transparent (Rahman *et al.*, 2016).

3.4.5 Conductivity - Conductivity is an optoelectronic event where the conductivity rises due to absorbing of photons. It provides the information about a material will be semiconductor, conductor or insulator. The photo conductivity spectrum of SrCo₂Si₂ shows in **Fig 4(e)**. From **Fig 4(e)** it is obvious that the photoconductivity starts with zero photon energy which also ensures the metallic nature of this compound. The photoconductivity of SrCo₂Si₂ increases due to the absorbing of photons (Sun *et al.*, 2006). From **Fig 4(e)** we have seen that the photoconductivity spectra have a few maxima and minima peak in the calculated energy range.

3.4.6 Loss function - The photon energy loss spectrum of SrCo₂Si₂ is shown in **Fig 4(f)**. The energy loss function is a significant matter to reveal the energy loss of a fast electron when it traversed in a material (Parvin *et al.*, 2015). In loss function graph the peaks related with the plasma resonance and in which associated frequency is called the plasma frequency ω_p (Fox, 2002). The frequency connected to the upper limit of the energy loss spectrum is specified by the bulk plasma frequency ω_p of the material, which emerges at $\epsilon_2 < 1$ and $\epsilon_1 = 0$ (Saniz *et al.*, 2006; Almeida *et al.*, 2006). The peak in the energy-loss function arises when $\epsilon_1(\omega)$ goes through zero from below and $\epsilon_2(\omega)$ goes through zero from above. In the energy loss spectra we have seen that the effective plasma frequency of SrCo₂Si₂ is equal to 14.42 eV. The highest peak is found at about 4.42 eV, which reveal the plasma frequency of SrCo₂Si₂. The material becomes transparent when the frequency of the incident light is higher than of plasma frequencies mentioned above. Furthermore, the peak in loss function corresponds to the trailing edges in reflection spectra.

4. CONCLUSION:

The different physical features such as mechanical, electronic and optical properties of intermetallic SrCo₂Si₂ have been successively investigated by DFT simulation. The investigated optimized structural parameters are well accord with the available synthesized data. The calculated elastic constants have maintained the born stability criteria which ensure the theoretical mechanical stability of SrCo₂Si₂. The calculated values of Pugh's ratio (B/G) and Poisson's ratio ensure the brittle nature of SrCo₂Si₂. The stiffer behavior of this phase is ensured by Young's modulus calculation. The analysis of universal anisotropic factor ensured the anisotropic nature of SrCo₂Si₂. The calculated band structure shows the metallic nature and major the part arrives from the Sr-4p states at Fermi level. High reflectivity is observed in the ultraviolet region energy site which ensure about the use of SrCo₂Si₂ as a good coating material at ultraviolet energy region. The absorption quality is good in the ultraviolet region and high refractive index in the infrared region. This result ensured that this compound is promising for absorbing materials in the UV region. The effective plasma frequency of SrCo₂Si₂ is found to 14.42 eV which ensures that this material becomes transparent when the frequency of the incident photon is higher than 14.42 eV.

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6. CONFLICTS OF INTEREST:

The authors declared that there is no conflict of interest in this article.

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