The Physical Properties of ThCr$_2$Si$_2$-Type Co-based Compound SrCo$_2$Si$_2$:
An ab-initio Study

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ABSTRACT

In this article, we have studied the mechanical, electronic, and optical features of ThCr$_2$Si$_2$-type compound SrCo$_2$Si$_2$. 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$_2$Si$_2$. The universal anisotropic constant $A_U$ ensures the anisotropic behavior of SrCo$_2$Si$_2$. The softness nature of SrCo$_2$Si$_2$ 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$_2$Si$_2$. 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$_2$Si$_2$.

Keywords: Co-based compound SrCo$_2$Si$_2$, Structural properties, Electronic properties, and Optical properties.

1. INTRODUCTION:

ThCr$_2$Si$_2$ type ternary intermetallic materials usually hold a superconducting ground position. The rare-earth AM$_2$X$_2$ structural materials have received great interest of researchers because of their many rich characteristics. Recently AM$_2$X$_2$ (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$_2$X$_2$ 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$_2$Si$_2$ 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$_2$Si$_2$-type structures are represented by Just and Paufler, (1996).

In recent times ThCr$_2$Si$_2$-type structure has gained massive consideration of researchers after discovering a new superconductor (Ba$_{0.3}$K$_{0.7}$) Fe$_2$As$_2$ belongs to the “122” family of iron-arsenide’s with ThCr$_2$Si$_2$ type structure exhibits high transition tem-
temperature 38K (Rotter et al., 2008). On the other hand, Pt, Ni and Pd-based ThCr$_2$Si$_2$ 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$_2$Si$_2$ type structure as example AFe$_2$As$_2$ (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 AFe$_2$X$_2$ compounds (Ae = alkaline earth metal, T = Ni, Pd; X = P, Ge) with very low transition temperatures (T$_c$ ∼ 0.3 - 3.0 K) (Mine et al., 2008). Undoped RT$_2$Si$_2$ (R = La, Y, Th; T = Ir, Pt) type superconductors are predicted to CaBe$_2$Ge$_2$-type structures (Yang et al., 2011). However the compounds with alkaline earth metals having ThCr$_2$Si$_2$-type structure are inadequate (Ronning et al., 2009; Fujii and Sato, 2009; Shelton et al., 1984; Doerrschmidt 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$_2$Si$_2$-type structure are inadequate. The compound SrCo$_2$Si$_2$ signifies the third ternary SrT$_2$Si$_2$ compound (T = 3d-block transition metals) besides SrCu$_2$Si$_2$ (Kranenberg et al., 2002) and SrZn$_2$Si$_2$ (May and Schäfer, 1972). For SrT$_2$Si$_2$ the isostructural compounds with T = Pd, Ag have been characterized and reported (Eisenmann et al., 1970). The compound SrCo$_2$Si$_2$ is isoelectronic to the parent Fe-pnictide superconductors AFe$_2$As$_2$ 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$_2$Si$_2$ 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$_2$Si$_2$. The calculations were done by DFT theory within GGA with the PBE exchange-correlation function (Clark et al., 2005; Materials Studio CASTEP, 2010; Hohenberg and Kohn, 1964; Perdew et al., 2008). The pseudo atomic calculations were done for Sr-4s$^2$ 4p$^6$ 5s$^2$, Si-3s$^2$ 3p$^2$ and Co-3d$^7$ 4s$^2$ 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$_2$Si$_2$. The crystal structure of SrCo$_2$Si$_2$ 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$_2$Si$_2$ were obtained by the stress-strain method (Fan et al., 2006). Then the bulk properties were obtained by the elastic constant data of SrCo$_2$Si$_2$. 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$_2$Si$_2$.

3. RESULT AND DISCUSSION:
3.1 Structural properties - At normal temperature and pressure, SrCo$_2$Si$_2$ 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$_2$Si$_2$ 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$_2$Si$_2$ 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$_2$Si$_2$](www.universepg.com)
Table 1: The calculated equilibrium lattice parameters, unit cell volume, bulk modulus of ThCr$_2$Si$_2$-type SrCo$_2$Si$_2$ compound in comparison with available experimental data.

| Properties | SrCo$_2$Si$_2$ | Deviation from Expt. (%) |
|------------|----------------|--------------------------|
| $a_0$ (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 SrCo$_2$Si$_2$ 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 SrCo$_2$Si$_2$ 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 SrCo$_2$Si$_2$ are listed in Table 2. According to the stability criteria (Pukunov et al., 2004) of tetragonal phase (Eq. 1) the compounds under consideration have good stability in nature.

$$C_{11}>0, \ C_{33}>0, \ C_{66}>0, \ C_{44}>0$$

$$2(C_{11}+C_{12})+4C_{13}+3C_{33}>0$$

(1)

Table 2: The evaluated elastic constants $C_{ij}$ (in GPa) of SrCo$_2$Si$_2$ 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 et al., 2019 |
| SrRh$_2$Ge$_2$ | 179.5   | 72.4     | 52.2     | 103.6    | 52.6     | 80.9     | Salma et al., 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 $\nu$ of intermetallic SrCo$_2$Si$_2$ 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.

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

(2)

$$B_R = C^2/M$$

(3)

$$G_V = M + 3C_{11} - 3C_{12} + 12C_{44} + 6C_{66} / 30$$

(4)

$$G_R = \frac{15}{C^{15}_V} + \frac{6}{C_{11}-C_{12}} + \frac{6}{C_{44}} + \frac{3}{C_{66}}$$

(5)

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

$$M = C_{11}+C_{12}+2C_{33}+4C_{13}$$

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.

$$B_H = B = \frac{1}{2}(B_R + B_V)$$

(6)
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, 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$_2$Si$_2$ is larger than SrRu$_2$As$_2$ and SrRh$_2$Ge$_2$ compounds indicating that the compound SrCo$_2$Si$_2$ is stiffer than SrRu$_2$As$_2$ and SrRh$_2$Ge$_2$ 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 (ν = 0.1) indicates the covalent materials whereas for ionic crystal ν = 0.25. The larger value of Poisson’s ratio (ν > 0.26) indicates that the compound will be ductile and the compound will be brittle when the value of Poisson’s ratio is (ν < 0.26). From Table 3, we see that the value of ν is 0.18 which refers the brittle nature of SrCo$_2$Si$_2$. 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$_2$Si$_2$ shows brittle manner which is very similar to Poisson’s ratio.

Table 3: Evaluated polycrystalline bulk modulus B (GPa), shear modulus G (GPa), B/G value, Poisson’s ratio ν and elastic anisotropy $A^U$ of SrCo$_2$Si$_2$ with similar types of compounds.

| Compounds | B    | G    | Y    | B/G  | ν    | $A^U$ | Ref.     |
|-----------|------|------|------|------|------|-------|---------|
| SrCo$_2$Si$_2$ | 80.60 | 64.44 | 152.64 | 1.25 | 0.18 | 0.629 | This work |
| SrRu$_2$As$_2$ | 86.11 | 55.03 | 136.05 | 1.56 | 0.23 | 0.180 | Chowdhury et al., 2019 |
| SrRh$_2$Ge$_2$ | 86.60 | 54.40 | 134.70 | 1.59 | 0.24 | 0.469 | Salma et al., 2018 |

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

\[
A^U = \frac{5G^2}{G_R} + \frac{B_v}{B_R} - 6 \quad (10)
\]

$A^U = 0$ 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$_2$Si$_2$ 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 SrCo$_2$Si$_2$ signifies that this compound might be superconductor. The partial and total density of states of SrCo$_2$Si$_2$ is plotted in Fig 3. From Fig 3 we have observed that the total density of states (TDOS) of SrCo$_2$Si$_2$ is composed of four main peaks.

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Fig 2: The band structure of compound SrCo$_2$Si$_2$.

The first peak in the valence band lies between -36.17 eV and -34.75 eV. In SrCo$_2$Si$_2$, Sr-5s states contribute the most to create the first peak. The second peak lies between -18.63 eV and -16.93 eV in SrCo$_2$Si$_2$. 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 SrCo$_2$Si$_2$, which suggests the covalent nature of Co-Si bonds in SrCo$_2$Si$_2$ (Rahman et al., 2016). This is a common feature of ThCr$_2$Si$_2$ 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 SrCo$_2$Si$_2$ with different photon energies are calculated by the frequency dependent dielectric function, \( \varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega) \), which is closely correlated to the electronic configurations. The imaginary part \( \varepsilon_2(\omega) \) 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):

\[
\varepsilon_2(\omega) = \frac{2e^2}{\Omega_0} \sum_{l,m} \left| \langle \psi_l^0 | \mathbf{u} \cdot \mathbf{\hat{r}} | \psi_m^c \rangle \right|^2 \delta(E^c_l - E^v_m - E)
\]

Where, \( \omega \) refers to light frequency, \( e \) indicates the electronic charge, \( \mathbf{u} \) is the vector representing the polarization of the incident electric field, along with \( \psi_l^0 \) and \( \psi_m^c \) are the conduction band and valence band wave functions at \( k \), successively. From the imaginary part \( \varepsilon_2(\omega) \), the real part \( \varepsilon_1(\omega) \) of the dielectric function is obtained through the Kramers-Kronig relations.

\[
\varepsilon_1(\omega) = 1 + \frac{2}{\pi} P \int_0^\infty \frac{\omega \varepsilon_2(\omega)}{\omega^2 - \omega^2} d\omega.
\]

Where, \( \omega \) 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).

\[
R(\omega) = \frac{\sqrt{\varepsilon(\omega) - 1}^2}{\sqrt{\varepsilon(\omega) + 1}^2}
\]

We calculate the absorption coefficient \( I(\omega) \), the real part of optical conductivity \( \text{Re}[\sigma(\omega)] \) and the elec-
electron energy-loss spectrum $L(\omega)$ using the following expressions (Delin et al., 1996).

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

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

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

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

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

The photon energy dependent ground state optical properties of SrCo$_2$Si$_2$ 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 Gaussian 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 multilayers. The optical reflectivity spectra are shown in Fig 4(a) as a function of incident photon energy. For SrCo$_2$Si$_2$ 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 wavelength 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 SrCo$_2$Si$_2$ 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.

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 SrCo$_2$Si$_2$ which is one of the important optical properties. In the low energy region the highest refractive index of SrCo$_2$Si$_2$ 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 \( \varepsilon_1(\omega) \) and imaginary \( \varepsilon_2(\omega) \) part of dielectric function of \( \text{SrCo}_2\text{Si}_2 \). The static value of dielectric constant is 40.80. The real part \( \varepsilon_1(\omega) \) goes to below from zero and back to zero up to 46.72 eV. The imaginary part for compound \( \text{SrCo}_2\text{Si}_2 \) 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 \( \text{SrCo}_2\text{Si}_2 \), 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 \( \text{SrCo}_2\text{Si}_2 \) 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 \( \text{SrCo}_2\text{Si}_2 \) 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 \( \text{SrCo}_2\text{Si}_2 \) 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 \( \omega_p \) (Fox, 2002). The frequency connected to the upper limit of the energy loss spectrum is specified by the bulk plasma frequency \( \omega_p \) of the material, which emerges at \( \varepsilon_2 < 1 \) and \( \varepsilon_1 = 0 \) (Saniz et al., 2006; Almeida et al., 2006). The peak in the energy-loss function arises when \( \varepsilon_2(\omega) \) goes through zero from below and \( \varepsilon_1(\omega) \) goes through zero from above. In the energy loss spectra we have seen that the effective plasma frequency of \( \text{SrCo}_2\text{Si}_2 \) is equal to 14.42 eV. The highest peak is found at about 4.42 eV, which reveal the plasma frequency of \( \text{SrCo}_2\text{Si}_2 \). 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 \( \text{SrCo}_2\text{Si}_2 \) 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 \( \text{SrCo}_2\text{Si}_2 \). The calculated values of Pugh’s ratio (B/G) and Poisson’s ratio ensure the brittle nature of \( \text{SrCo}_2\text{Si}_2 \). The stiffer behavior of this phase is ensured by Young’s modulus calculation. The analysis of universal anisotropic factor ensured the anisotropic nature of \( \text{SrCo}_2\text{Si}_2 \). The calculated band structure shows the metallic nature and major the part arrives from the \( \text{Sr-}4p \) states at Fermi level. High reflectivity is observed in the ultraviolet region energy site which ensure about the use of \( \text{SrCo}_2\text{Si}_2 \) 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 \( \text{SrCo}_2\text{Si}_2 \) 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.

7. REFERENCES:
1) Ali M.L., Rahman M. Z. and Rahman M.A., (2016). The structural, elastic and optical properties of ScM (M= Rh, Cu, Ag, Hg) intermetallic compounds under pressure by \textit{ab initio} simulations. International J. of Computational Materials Science and Engineering, 5(04), p.1650024. https://arxiv.org/abs/1602.03152
2) Ali M.S., Ali M.A., Parvin R. and Islam A.K. M.A., (2016). New MAX phase compound \( \text{Mo}_2\text{TiAlC}_2 \): first-principles study. arXiv preprint arXiv:1603.04215.
3) Ban Z. and Sikirica M., (1965). The crystal structure of ternary silicides ThM3Si2 (M = Cr, Mn, Fe, Co, Ni and Cu). Acta Crystallographica, 18(4), pp.594-599.

4) Bodak O.I., and Gladyshevskii E.I., (1968). X-ray diffraction investigation of the system Ca-Ni-Si and alloys of related systems. Dopov. Akad. Nauk. Ukr. RSR, 30, pp.944-947. https://arxiv.org/ftp/arkiv/papers/1210/1210.7613.pdf

5) Cao Y., Zhu J., and Lai Z., (2013). First principles studies of the structural, elastic, electronic and thermal properties of Ni3Si. Computational materials science, 69, pp.40-45.

6) Cava R.J., Batlogg B., and Van Dover R.B., (1994). Superconductivity in RPt3B3C. Physical Review B, 49(17), p.12384. https://doi.org/10.1103/PhysRevB.49.12384

7) Cava R.J., Takagi H., Kra-jewski J.J., and Lee J.O., (1994). Superconductivity in the quaternary intermetallic compounds LnNi3B3C. Nature, 367(6460), 252-253.

8) Chen X.Q., Niu H., Li, D. and Li Y., (2011). Modeling hardness of polycrystalline materials and bulk metallic glasses. Intermetallics, 19(9), pp.1275-1281. https://doi.org/10.1016/j.intermet.2011.03.026

9) Chowdhury U.K., Rahman A., and Roy D.C., (2019). The physical properties of ThCr2Si2-type Ru-based compounds SrRu2X2 (X= P, Ge, As): An ab-initio investigation. Physica C: Superconductivity and its applications, 562, pp.48-55.

10) Chung D.H. and Buessem W.R., (1967). The elastic anisotropy of crystals. Journal of Applied Physics, 38(5), pp.2010-2012. https://doi.org/10.1063/1.1709819

11) Clark S.J., Segall M.D., and Payne M.C., (2005). First principles methods using CASTEP. Zeitschrift für kristallographie-crystalline materials, 220(5-6), pp.567-570.

12) De Almeida, J.S. and Ahuja R., (2006). Electronic and optical properties of RuO2 and IrO2. Physical Review B, 73(16), p.165102. https://doi.org/10.1103/PhysRevB.73.165102

13) Delin A., Eriksson O., Ahuja R., and Wills J. M., (1996). Optical properties of the group-IVB refractory metal compounds. Physical Review B, 54(3), p.1673. https://doi.org/10.1103/PhysRevB.54.1673

14) Doerrschmidt W., Niess N. and Schaefer H., (1976). New compounds of the ThCr2Si2-structure type. Z. Naturforsch., B, 31(6), 890-891.

15) Eisenmann B., May N., and Ziegleder G., (1970). Neue Vertreter des ThCr2Si2-Typs und dessen Verwandt schaftzum Anti-PbFCl-Gitter. Zeitschrift für Naturforschung B, 25(12), pp.1350-1352.

16) Fan C.Z., Zeng S.Y., and Yao Y.G., (2006). Potential superhard osmium dinitride with fluorite and pyrite structure: First-principles calculations. Physi. Review B, 74(12), p.125118. https://doi.org/10.1103/PhysRevB.74.125118

17) Fox M., (2001). Optical Properties of Solids New York: Oxford University press.

18) Fujii H. and Sato A., (2009). Superconductivity in SrPd3Ge2. Physical Rev. B, 79(22), p.224522. https://doi.org/10.1103/PhysRevB.79.224522

19) Golesorkhtabar R., Pavone, P., and Draxl C., (2013). ElaStic: A tool for calculating second-order elastic constants from first principles. Computer Physics Communicat., 184(8), pp.1861-1873.

20) Hill R., (1952). The elastic behaviour of a crystalline aggregate. Proceedings of the Physical Society. Section A, 65(5), p.349. https://iopscience.iop.org/article/10.1088/0370-1298/65/5/307/meta

21) Hoffmann A.V., Hlukhyy V. and Fässler T.F., (2012). Synthesis and structure of SrCo2Si2 and CaRh3Si2-isoelectronic variants of the parent superconductors AeFe2As2 and study of the influence of the valence electron count in CaFe2,Rh3Si2. arXiv preprint arXiv:1210.7152

22) Hohenberg P. and Kohn W., (1964). Phys. Rev. 136(1964); B864–B871. https://doi.org/10.1103/PhysRev.136.B864

23) Hu W.C., Liu Y., and Xu C.S., (2014). First-principles study of structural and electronic properties of C14-type Laves phase Al2Zr and Al2Hf. Comput. Materials Sci., 83, pp.27-34. http://dx.doi.org/10.1016/j.commatsci.2013.10.029

24) Imada M., Fujimori A. and Tokura Y., (1998). Metal-insulator transitions. Reviews of modern physics, 70(4), p.1039. https://doi.org/10.1103/RevModPhys.70.1039

25) Jeitschko W., Glau R. and Boonk L., (1987). Superconducting LaRu2P2 and other alkaline earth and rare earth metal ruthenium and os-
mium phosphides and arsenides with ThCr$_2$Si$_2$ structure. *J. of solid state chem.*, 69(1), 93-100.

26) Johnston D.C., (2010). The puzzle of high temperature superconductivity in layered iron pnictides and chalcogenides. *Advances in Physics*, 59(6), pp.803-1061. https://doi.org/10.1080/00018732.2010.513480

27) Just, G. and Paaufler, P., (1996). On the coordination of ThCr$_2$Si$_2$ BaAl$_2$-type compounds within the field of free parameters. *Journal of alloys and compounds*, 232(1-2), pp.1-25.

28) Koç H., Mamedov A.M., Deligoz E. and Ozisik H., (2012). First principles prediction of the elastic, electronic, and optical properties of Sb$_2$Se$_3$ and Sb$_2$Se$_5$ compounds. *Solid State Sciences*, 14(8), pp.1211-1220. https://doi.org/10.1016/j.solidstatesciences.2012.06.003

29) Kranenberg C., Trill H. and Mosel B.D., (2002). New compounds of the ThCr$_2$Si$_2$-type and the electronic structure of CaM$_2$Ge$_3$ (M: Mn–Zn). *J. of Solid-State Chemistry*, 167(1), pp.107-112.

30) Materials Studio CASTEP manual_Accelrys, (2010). pp. 261–262. http://www.tcm.phy.cam.ac.uk/castep/document/CASTEP.html

31) May N. and Schäfer H., (1972). Neue Verbindungenim ThCr$_2$Si$_2$-Typ/New Compounds in the ThCr$_2$Si$_2$-Type. *Zeitschrift für Natur für schung B*, 27(7), pp.864-865.

32) Mine T., Yanagi H. and Hosono H., (2008). Nickel-based phosphide super conductor with infinite-layer structure, BaNi$_2$P$_2$. *Solid state communications*, 147(3-4), pp.111-113. https://doi.org/10.1016/j.ssc.2008.05.010

33) Monkhorst H.J. and Pack J.D., (1976). Special points for Brillouin-zone integrations. *Physical review B*, 13(12), p.5188.

34) Mostari F., Rahman MA, and Khatun R. (2020). First principles study on the structural, elastic, electronic and optical properties of cubic ‘half-Heusler’ alloy RuVAs under pressure, *Int. J. Mat. Math. Sci.*, 2(4), 51-63. https://doi.org/10.34104/ijmms.020.051063

35) Nagarajan R., Hossain Z., Dhar S.K., Vijayaraghavan R., (1994). Bulk superconductivity at an elevated temperature (T_c ≈ 12 K) in a nickel containing alloy system Y-Ni-BC. *Physical review letters*, 72(2), p.274. https://doi.org/10.1103/PhysRevLett.72.274

36) Nye J.F., (1961). Properties Physiques des Materiaux. *Dunod, Paris.*

37) Palenzona A., Cirafici S. and Canepa F., (1987). High temperature behaviour of unstable EuPd$_2$Si$_2$ and reference MPd$_2$Si$_2$ compounds (M = All rare earths and alkaline earths). *J. of the Less Common Metals*, 135(2), pp.185-194. https://doi.org/10.1016/0022-5088(87)90479-6

38) Parvin F., M. A. and A. K. Islam M. A., (2015). "Mechanical, electronic, optical, thermodynamic properties and superconductivity of ScGa$_3$." *Physica B: Condensed Matter* 457; 320-325

39) Perew J.P., Csonka G.I., Zhou X. and Burke K., (2008). Restoring the density-gradient expansion for exchange in solids and surfaces. *Physical review letters*, 100(13), p.136406. https://doi.org/10.1103/PhysRevLett.100.136406

40) Pfommer B.G., Côté M., Louie S.G. and Cohen M.L., (1997). Relaxation of crystals with the quasi-Newton method. *Journal of Computational Physics*, 131(1), pp.233-240. https://doi.org/10.1006/jcph.1996.5612

41) Piskunov S., Eglitis R.I. and Borstel G., (2004). Bulk properties and electronic structure of SrTiO$_3$, BaTiO$_3$, PbTiO$_3$ perovskites: an ab initio HF/DFT study. *Computational Materials Science*, 29(2), pp.165-178.

42) Pugh S.F., (1954). XCIII. Relations between the elastic moduli and the plastic properties of polycrystalline pure metals. The London, Edinburgh, and Dublin Philosophical Magazine and J. of Science, 45(367), pp.823-843. https://doi.org/10.1080/14786440808520496

43) Rahman M.A., Rahaman M.Z. and Sarker M.A.R., (2016). First principles investigation of structural, elastic, electronic and optical properties of HgGeB$_2$ (BP, As) chalcopyrite semiconductors. *Computat. Condensed Matter*, 9, pp.19-26. https://doi.org/10.1016/j.cocom.2016.09.001

44) Rahaman M.Z. and Rahman M.A., (2016). Novel Laves phase superconductor NbBe$_2$: A theoretical investigation. *Comput. Condensed Matter*, 8, pp.7-13. https://doi.org/10.1016/j.cocom.2016.06.001

45) Rahman M.A., Rahaman M.Z. and Rahman M.A., (2016). The structural, elastic, electronic and optical properties of MgCu under pre-
Superconducting Fe-based compounds (A = K and Cs with transition temperatures up to 37 K. Superconductivity at 38 K in the iron arsenide (Ba$_{1-x}$K$_x$) Fe$_2$As$_2$. Physical Review Letters, 101(10), p.107006.

50) Russell P., (2003). Photonic crystal fibers. Science, 299(5605), pp.358-362. https://doi.org/10.1126/science.1079280

51) Salma M.U. and Rahman M.A., (2018). Physical properties of ThCr$_2$Si$_2$-type Rh-based compounds A Rh$_2$Ge$_2$ (A= Ca, Sr, Y and Ba): DFT based first-principles investigation. Intern. J. of Modern Phys. B, 32(32), 1850357.

52) Saniz R., Ye L.H., and Freeman A.J., (2006). Structural, electronic, and optical properties of NiAl$_2$: first-principles calculations. Physical Review B, 74(1), p.014209. https://doi.org/10.1103/PhysRevB.74.014209

53) Sasmal K., Lv B., and Chu C.W., (2008). Superconducting Fe-based compounds (A$_{1-x}$Sr$_x$) Fe$_2$As$_2$ with A = K and Cs with transition temperatures up to 37 K. Physical Review Letters, 101(10), p.107007. https://doi.org/10.1103/PhysRevLett.101.107007

54) Segall M.D., Lindan P.J., and Payne M.C., (2002). First-principles simulation: ideas, illustrations and the CASTEP code. Journal of physics: condensed matter, 14(11), p.2717.

55) Shelton R.N., Brau H.F. and Musick E., (1984). Superconductivity and relative phase stability in 1: 2 ternary transition metal sili- cides and germanides. Solid state communications, 52(9), pp.797-799. https://doi.org/10.1016/0038-1098(84)90008-5

56) Stewart G.R., (2001). Non-Fermi-liquid behavior in d-and f-electron metals. Reviews of modern Physics, 73(4), p.797.

57) Stewart G.R., (2011). Superconductivity in iron compounds. Reviews of Modern Physics, 83(4), p.1589. https://doi.org/10.1103/RevModPhys.83.1589

58) Sun J., Zhou X.F., and Tian Y., (2006). Pressure induced superconductivity in CaFe$_2$As$_2$. Physical review letters, 101(5), p.057006. https://doi.org/10.1103/PhysRevLett.101.057006

59) Torikachvili M.S., Ni N. and Canfield P.C., (2008). Pressure induced superconductivity in CaFe$_2$As$_2$. Physical review letters, 101(5), p.057006. https://doi.org/10.1103/PhysRevLett.101.057006

60) Villars, P. and Cenzual, K., (2007). Pearson’s Crystal Structure Database for Inorganic Compounds (on CD-ROM), 1. Materials Park, OH, (USA), 8.

61) Yang C.D., ChenY.Y., and Hsu Y.Y., (2011). Superconductivity in Sr (Pd$_{1-x}$Ni$_x$)$_2$Ge$_2$. In J. of Physics: Conference Series, 273(1), pp. 012089.

62) Zhu Y.D., Yan M.F., and Zhang C.S., (2016). First-principles investigation of structural, mechanical and electronic properties for Cu-Ti intermetallics. Comput. Material. Sci., 123, pp. 70-78. https://doi.org/10.1016/j.commatsci.2016.06.015

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