

Structural, electronic, mechanical, and dynamical properties of scandium carbide

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ABSTRACT

We report results of first-principles calculations for the structural, mechanical, dynamical and electronic properties of Scandium Carbide (ScC) compound, using a Full-Potential Linearized-Augmented Plane Wave (FP-LAPW) method based on density functional theory, within the generalized gradient approximation (GGA). The computed ground states properties; lattice constants, bulk modulus and the pressure derivative of the bulk modulus (a_0 , B and B') are in good agreement with former works. The calculated transition pressures from the rocksalt (NaCl) structure to the CsCl structure and from the NiAs to CsCl are found to be 111.0 GPa and 27.15 GPa, respectively. It was found, that NaCl and NiAs are mechanically and dynamically the stable phases, with NaCl considered as the ground state phase. In contrast, the Zincblende (ZB) and CsCl are both unstable phases mechanically and dynamically. Wurtzite (WZ) phase was found mechanically stable and dynamically not, which might be a possible indication for a metastable phase. The electronic structures reveal that all the considered structures have a metallic character. Upon our best knowledge, for the first time, the mechanical and dynamical properties of the studied structures beside NaCl were calculated.

Introduction

Recently, first principles-based methods (ab initio methods) which use only the atomic constants as input parameters for solving the Schrödinger equation have now become the most powerful probes for computing with a great accuracy an important number of structural and electronic properties of solids. Among the quantities obtained from this kind of study are the crystal structure, lattice constant, bulk and shear moduli and other static and dynamical properties. Needless to mention that they are also a tool of choice for the prediction of new materials, and they could sometimes replace experiments which are very costly or even impossible in the laboratory.

The high-pressure structural behavior of binary *AB* compounds has been a popular topic in condensed matter research. The majority of these compounds undergo the first order structural phase transition from

NaCl-type (*B1*) to *CsCl*-type (*B2*) structure at high pressure. There have been considerable works involving both experimental and theoretical methods on the structural phase transition and elastic constants in *AB* compounds such as the rare-earth, lanthanides and actinides Chalcogenides and Pnictides [1-19]. Among *AB* compounds, the metal carbides have interesting physical and chemical properties, such as metallic conductivity, high melting point and hardness. Because of their properties and their potential applications, metal carbides have gained a high interest and have been a subject of some theoretical and experimental studies. The low density of state (DOS) at Fermi-Level for the NaCl structure was predicted by Zhang et al. in 2002 [20]. The metallic character of the rocksalt (NaCl) ScC was found by Maibam et al. in 2011 and Soni et al. in 2012 [21,22]. Later Soni et al. calculated the phase transition pressure from the NaCl to CsCl and found it to be 127.8 GPa, using the full potential plane wave (FP-LAPW) method [23]. Rahim and

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Table 1

Coordinates of the Anion and Cation with their number of special k-points of ScC for each structure.

| Structure | Space Group | Cation (Sc) Coordinates | Anion (C) Coordinates | No. of special k-points |
|-----------|-------------|-------------------------|-----------------------|-------------------------|
| RS | 225 Fm-3m | (0,0,0) | (1/2, 1/2, 1/2) | 286 |
| NiAs | 194 P63/mmc | (0,0,0) | (1/3, 2/3, 1/4) | 308 |
| WZ | 186 P63mc | (1/3, 2/3, 0) | (1/3, 2/3, u) | 308 |
| CsCl | 221 Pm-3m | (0,0,0) | (1/2, 1/2, 1/2) | 286 |
| ZB | 216 F-43 | (0,0,0) | (1/4, 1/4, 1/4) | 286 |

Table 2

Optimized structural properties of the cubic phases of ScC.

| Structure | | Lattice constant a (Å) | Volume V_0 (Bohr ⁻³) | Bulk Modulus B (GPa) | First Derivative B' |
|-------------|--------------|--------------------------|------------------------------------|----------------------|---------------------|
| RS | Present Work | 4.6355 | 168.0484 | 164.2023 | 3.8680 |
| | Others | 4.680 [27], | 172.82 [26] | 153 [27] | |
| | | 4.682 [23], | 172.96 [27] | 155 [23] | 3.36 [23] |
| | | 4.689 [24], | 173.16 [23] | 157 [24] | 3.76 [24] |
| | | 4.668 [28], | 173.90 [24] | 150 [28] | |
| | | 4.678 [26], | 171.61 [28] | 152 [26] | 3.98 [26] |
| | | 4.637* [29], | 168.24 [29] | | |
| 4.720* [30] | 177.41 [30] | | | | |
| CsCl | Present Work | 2.8420 | 159.9141 | 158.1676 | 4.3607 |
| | Others | 2.876 [23], | 160.20 [26] | 149 [23] | 4.01 [23] |
| | | 2.874 [26], | 160.54 [23] | 149 [26] | 4.00 [26] |
| | | 2.889 [24] | 162.63 [24] | 126 [24] | 3.74 [24] |
| ZB | Present Work | 5.0301 | 214.7205 | 106.6913 | 3.7769 |
| | Others | 5.085 [24] | 222.29 [24] | 99 [24] | 4.87 [24] |
| | | 5.075 [26] | 220.81 [26] | 89 [26] | 3.66 [26] |

* Experimental results.

Rodriguez claimed in 2013 that NiAs structure is the most stable phase for ScC and confirmed the phase transition from the NaCl to CsCl is occurred at 127 GPa [24]. The knowledge of elastic constants is very useful, as it gives information about the mechanical properties of a solid, such as internal strain, elastic anisotropy, and mechanical stability. Due to the absence of theoretical and experimental study of mechanical and dynamical stability of ScC compound and in order to study its structural phase stability in the different phases, we have performed first-principles calculation on the structural phase stability, electronic, mechanical, and lattice dynamical properties by using the state of the art full potential augmented plane wave (FP-LAPW) method, in the framework of the density functional theory (DFT) with the generalized gradient approximation GGA. This paper is structured as follows: In the second section the calculation method is described. The most relevant results are displayed and discussed in section three. In the last section, a conclusion of the main results is given.

Table 3

Optimized structural properties of the hexagonal structures of ScC.

| Structure | Lattice constant a (Å) | Lattice constant c (Å) | c/a | Internal parameter u | Volume V_0 (Bohr ⁻³) | Bulk Modulus B (GPa) | First Derivative B' |
|-----------|--------------------------|--------------------------|--------|------------------------|------------------------------------|----------------------|---------------------|
| WZ | 3.5596 | 5.3380 | 1.5531 | 0.39147 | 424.0911 | 112.3784 | 3.7153 |
| Others | 3.961 [26] | 4.563 [26] | | | | 113 [26] | 4.15 [26] |
| | 3.926 [24] | 4.556 [24] | | | | 116 [24] | 3.62 [24] |
| | 3.3667 | 6.0257 | 1.8678 | - | 348.6974 | 148.2489 | 3.5531 |
| NiAs | 3.208 [26] | 5.970 [26] | | | | 53.20 | 3.80 [26] |
| | 3.487 [24] | 4.868 [24] | | | | [26] | 3.58 [24] |
| | | | | | | 51.33 [24] | |

Computational details

The calculations in the present study were carried out by using the WIEN2k computer package utilizing the Full-Potential Linearized-Augmented Plane Wave (FP-LAPW) method, considered to be one of the most accurate approaches for the ground state properties. The exchange correlation effect was treated by the Perdew-Burke-Ernzerhof generalized gradient approximation (PBE-GGA) [25]. In FP-LAPW method each unit cell is divided into muffin tin (MT) spheres centered on each atom and interstitial region. We considered R_{MT} of 2.00 and 1.88 atomic units (a. u.) for Sc and C atoms, respectively. In the calculations of the cubic structures a $21 \times 21 \times 21$ mesh of points with a total amount of 10000 k-points are used. For the hexagonal structure a mesh of $24 \times 24 \times 8$ k-points with a total amount of 5000 total k-points are used (see Table 1). The lattice parameters of each structure were optimized by minimizing the total energy with respect to the volume (and the internal parameter u in the WZ case).

Results and discussion

Structural properties

For obtaining the equilibrium structural parameters for the cubic structures, the total energy was minimized with respect to the unit cell volume (and therefore with respect to the lattice parameters). The energy versus volume curve is fitted by Murnaghan's equation of state (EOS) to calculate the ground state properties such as the equilibrium lattice constant (a), bulk modulus (B) and the first pressure derivative of bulk modulus (B'). The computed parameters of the cubic structures are displayed in Table 2 along with the previous theoretical results [23,24,26-28] and experimental data [29,30].

For the hexagonal structures we minimized the total energy related to the unit cell volume and the internal parameter u . Therefore, we first vary the ratio of the two lattice constants (c/a) to find the optimum ratio by minimizing the total energy. Involving the (c/a) constant, we calculated the optimized lattice constants a and c . We did the same procedure for optimizing the internal parameter u . When obtaining the optimized (c/a) and u , we were able to vary the volume versus energy to find the equilibrium structural parameters (a , c , B and B') with fitting to the Murnaghan's equation of state (EOS). The calculated parameters are displayed in Table 3 along with the previous theoretical results [24,26]. Compared with previous studies our results for the cubic structural parameters are in good agreement. There are differences in the (c/a) ratio values, for the hexagonal structures, although the lattice constant (a) is in good agreement. As far as we know, there are no available experimental results to compare with our results.

The equation of state (EOS) of each structure is plotted in Fig. 1. This indicates that the NaCl structure is the most stable. This is in agreement with the results of Zhao and co-workers [26] and disagrees with that of Rahim and Rodriguez [24] who claims that the NiAs structure is the ground state.

Fig. 1 shows that there are phase transitions from the ground state, NaCl-structure, to the other structures such as the CsCl. In Figs. 2 and 3 the enthalpy, $H = E + PV$, is plotted as a function of the pressure. The value of the structural phase transition pressure is determined by the

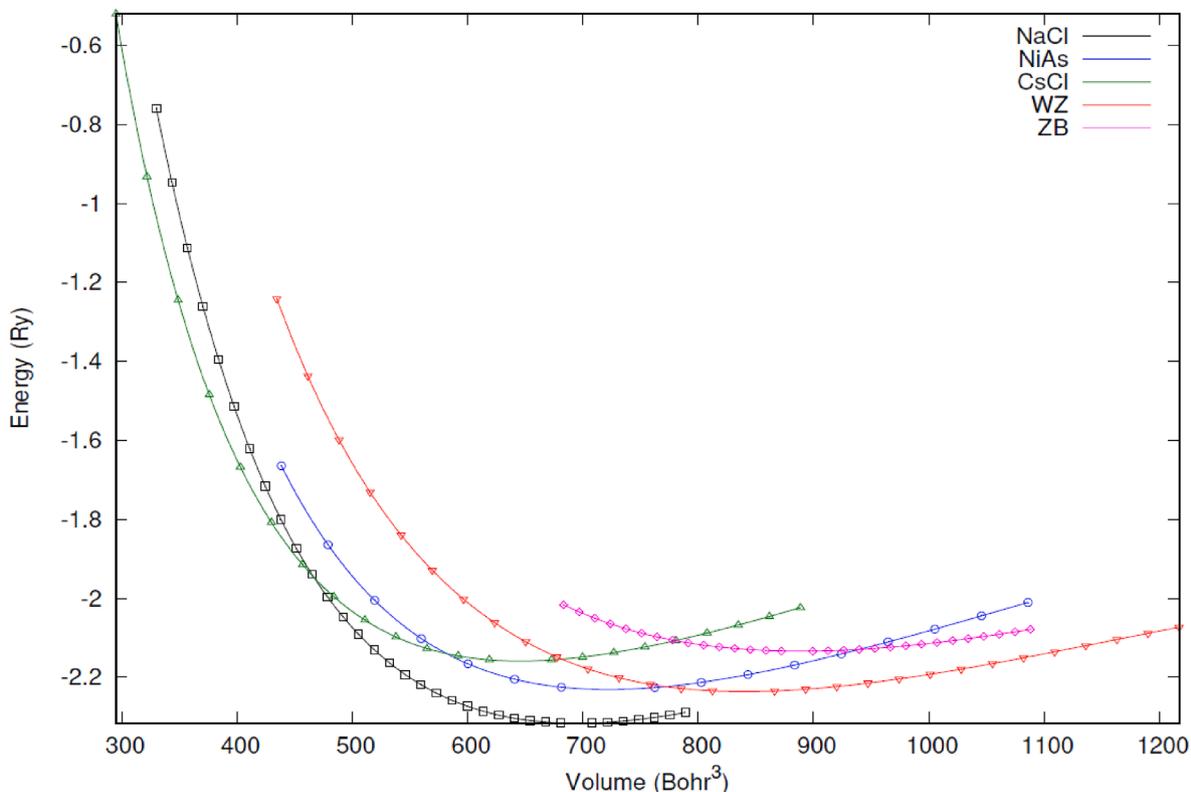


Fig. 1. Volume dependence of the electronic energy of ScC in the NaCl, NiAs, WZ, CsCl and ZB structures.

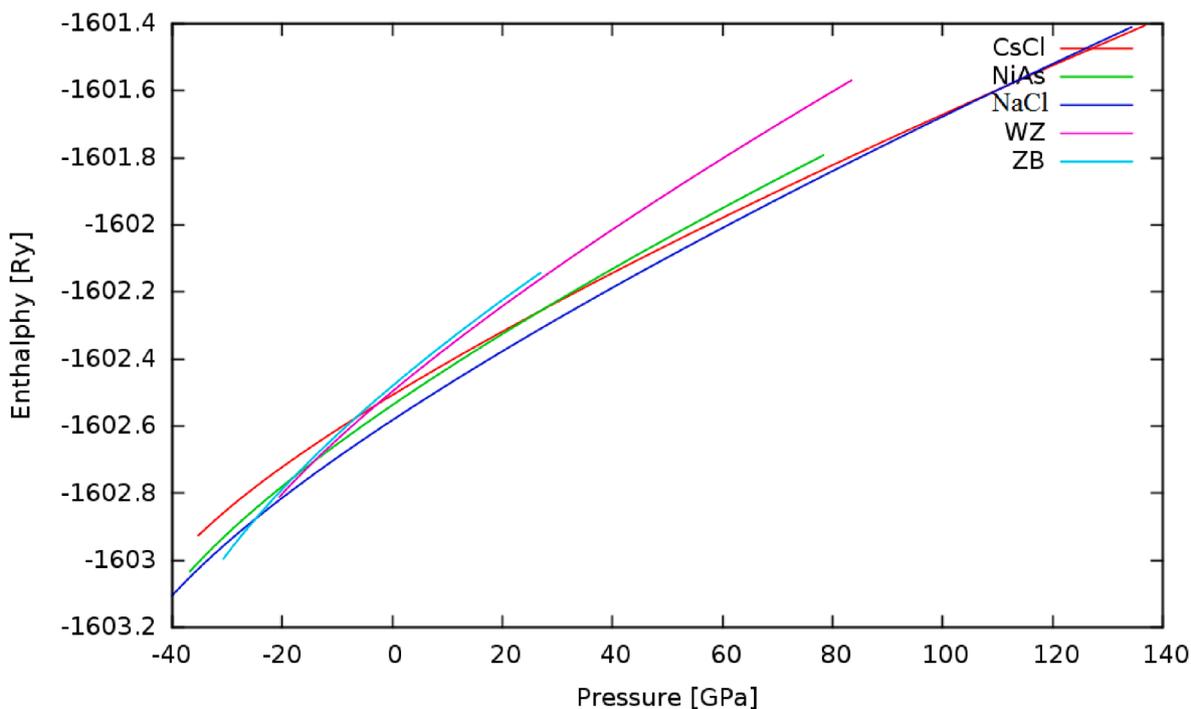


Fig. 2. Enthalpy as a function of pressure for ScC compound within all structures.

value of pressure, at which two structures have equal enthalpy.

The calculated pressures of all phase transitions are presented and compared with results of former work in Table 4 [24,26]. The difference between the results is due to the sensitivity of the phase transition to the method of calculation.

Fig. 3 (a & b) shows that a structural phase transitions from NaCl to

CsCl and NiAs to CsCl are occurred at about 111.0 GPa and 27.15GPa, respectively. Our results are comparable to the values of 108.9 GPa and 32 GPa obtained by Zhao and co-workers.

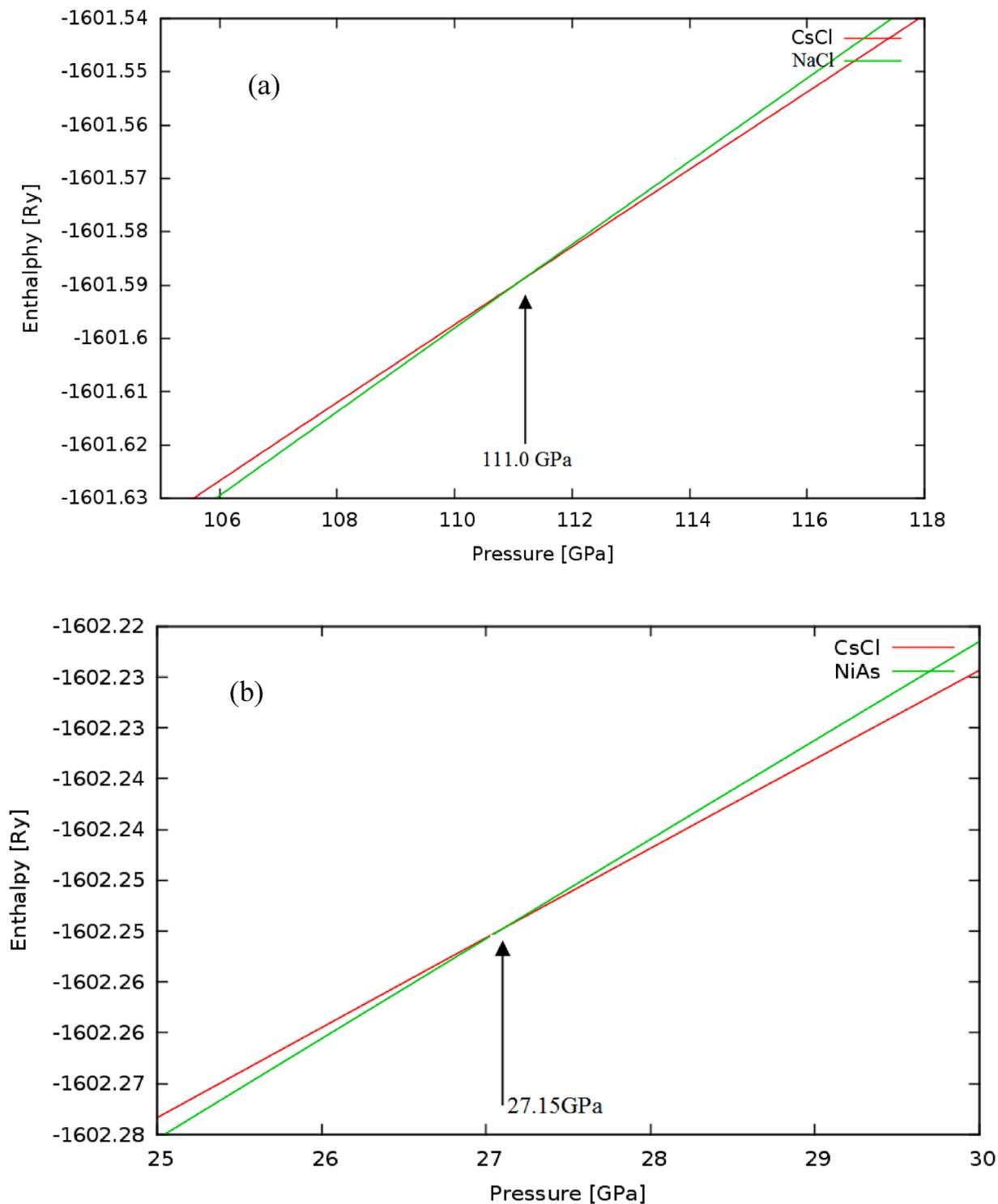


Fig. 3. Enthalpy as a function of pressure for ScC compound with a) CsCl and NaCl structures b) CsCl and NiAs structures.

Table 4

Transition pressure for different phase transitions.

| Structure | Present work P (GPa) | Other works P (GPa) |
|--------------|----------------------|----------------------------------|
| NiAs to CsCl | 27.15 | 32 [26], 12.7 [24] |
| RS to CsCl | 111.0 | 127.8 [23], 108.9 [26], 127 [24] |

Elastic properties

Beside the structural calculations, the elastic constants have been calculated using the optimized lattice parameters. Therefore, the stress, generated by forcing a small strain to an optimized unit cell, has been computed using the Cubic-elastic and Hex-elastic packages developed by Morteza Jamal [31].

The knowledge of the elastic constants is essential for the understanding of many phenomena of solids, like adjacent atomic planes bonding characteristics, structural stability, and anisotropic factor.

Table 5
Elastic constants of ScC for cubic and hexagonal structures (for hexagonal structures $C_{44} = C_{55}$).

| Structure | | C_{11} (GPa) | C_{12} (GPa) | $C_{44} = C_{55}$ (GPa) | C_{33} (GPa) | C_{13} (GPa) |
|-----------|--------------------|-------------------|----------------|----------------------------|----------------|-------------------|
| RS | Present Work | 337.58 | 68.27 | 60.55 | – | – |
| | Other calculations | 305 [26] | 76 [26] | 57 [26] | – | – |
| | | 305 [28] | 73 [28] | 46 [28] | – | – |
| | | 310 [23] | 77 [23] | 62 [23] | – | – |
| | | 313 [22] | 77 [22] | 64 [22] | – | – |
| CsCl | 83.65 | 188.64 | –109.14 | – | – | |
| ZB | 83.98 | 122.0539 | 75.66 | – | – | |
| NiAs | 207.28 | 142.0121 | 4.1352 | 284.8687 | 61.6316 | |
| WZ | 242.94 | 111.57 | 30.45 | 257.70 | 92.20 | |

Each cubic system has three independent elastic constants, namely C_{11} , C_{12} , and C_{44} . The hexagonal structures like NiAs structure is characterized by five elastic constants, C_{11} , C_{33} , C_{13} , C_{12} and C_{55} . The calculated elastic moduli are listed in Table 5 along with previous results for comparison [22,23,26,28]. Good agreement is found.

Once the elastic constants were determined one can conclude the stability of the structure based on the following cubic criteria:

$C_{11} > 0$, $C_{12} > 0$, $C_{44} > 0$, $C_{11} + 2 C_{12} > 0$, $C_{11} > B > C_{12}$ [32], where B is the bulk modulus.

Applying these criteria to our results, it appears that, out of all studied cubic structures, only the NaCl structure is stable because the elastic modulus C_{44} for CsCl structure has a negative value, while C_{12} is larger than C_{11} within ZB structure.

Similarly, the criteria for the hexagonal structure are, $C_{11} > |C_{12}|$, $C_{55} > 0$ [33]. It is concluded that the both NiAs and WZ are elastically stable. Compared with the equation of state (Fig. 1), we conclude that,

Table 6
Mechanical properties of ScC: Young’s modulus (Y), Bulk modulus (B), Shear’s modulus (S), Compressibility (β), Anisotropic ratio (A), Poisson’s ratio (ν), Transverse elastic wave velocity, Average wave velocity and Debye temperature.

| Structure | | RS | CsCl | ZB | NiAs | WZ |
|---|------------------------|-----------|----------|---------|---------|--------|
| Young’s modulus Y (GPa) | Present Work Others | 213.900 | –296.402 | –13.415 | 65.539 | 136.54 |
| | | 195 [26] | – | – | – | – |
| | | 176 [28] | – | – | – | – |
| | | 205 [23] | – | – | – | – |
| | | 208 [22] | – | – | – | – |
| Bulk modulus B (GPa) | Present Work Others | 158.045 | 153.643 | 102.699 | 136.663 | 148.39 |
| | | 152 [26] | – | – | – | – |
| | | 150 [28] | – | – | – | – |
| | | 155 [23] | – | – | – | – |
| | | 157 [22] | – | – | – | – |
| Shear’s modulus S (GPa) | Present Work Others | 83.920 | –81.361 | – 4.408 | 23.076 | 50.70 |
| | | 76 [26] | – | – | – | – |
| | | 67 [28] | – | – | – | – |
| | | 80 [23] | – | – | – | – |
| | | 82 [22] | – | – | – | – |
| Compressibility β (GPa^{-1}) | | 0.00633 | 0.0065 | 0.0097 | 0.0073 | 0.0067 |
| Anisotropic ratio A | Present Work Others | 0.4496 | – | – | 0.0448 | 0.385 |
| | | 0.50 [26] | – | – | – | – |
| | | 0.40 [28] | – | – | – | – |
| | | 0.53 [23] | – | – | – | – |
| | | 0.54 [22] | – | – | – | – |
| Poisson’s ratio ν | | 0.2386 | – | – | 0.4201 | 0.346 |
| Transverse elastic wave velocity (m/s) | | 4698.15 | – | – | 2740.8 | 3962.0 |
| Longitudinal elastic wave velocity (m/s) | | 8426. | 3309.54 | 5706.84 | 7382.7 | 8177.4 |
| Average wave velocity (m/s) | | 5231.08 | – | – | 3111.1 | 4452.6 |
| Debye temperature (K) | Present Work Others | 672.138 | – | – | 372.3 | 541.8 |
| | | 642 [26] | – | – | – | – |
| | | 665 [28] | – | – | – | – |
| | | 665 [23] | – | – | – | – |
| | | 748 [22] | – | – | – | – |

the NaCl structure is the ground state since it has the lowest minimum energy and is the most stable structure. Among all the studied structures, the NaCl structure is the more stable one. Moreover, the elastic constants of a system provide information about useful mechanical properties, such as brittleness/ductility, stiffness, hardness, bulk modulus (B), shear’s modulus (S), Young’s modulus (Y), compressibility (β), anisotropic ratio (A) and Poisson’s ratio (ν). The computed results along with the previous works [22,23,26,28] are presented in Table 6.

To evaluate these properties, two different methods of approximation can be used, the Voigt (V) approximation and the Reuss (R) method [34,35]. In addition, the elastic and mechanical properties can be estimated using the Voigt-Reuss-Hill expression, which is similar to the arithmetic mean of Reuss and Voigt [36].

The average compressibility can be found by calculating: $\beta = 1/B$, as the bulk modulus increased the compressibility decreased. The NaCl structure with a large bulk modulus has the lowest compressibility, while ZB has the largest compressibility.

The anisotropic ratio (A) is an indicator for the anisotropy of the average wave velocity of a crystal. It is equal to one for an anisotropy material. For cubic structures it is given by [37]:

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

On the other hand, for hexagonal systems, the anisotropy ratio (A) is calculated by [37]:

$$A = \frac{4C_{44}}{(C_{11} + C_{33} - 2C_{13})}$$

The material is completely isotropic for $A = 1$, variations of A defines the elastic anisotropy. According to this criterion, the NiAs structure with A approximately equals to 0.045 is completely anisotropic, in contrast to that, for the NaCl phase A equals nearly 0.5.

The Poisson’s ratio, can be computed as the following: $\nu = (3B-2S)/(6B + 4S)$.

The critical value of Poisson’s ratio is 0.26 according to Frantsevich’s

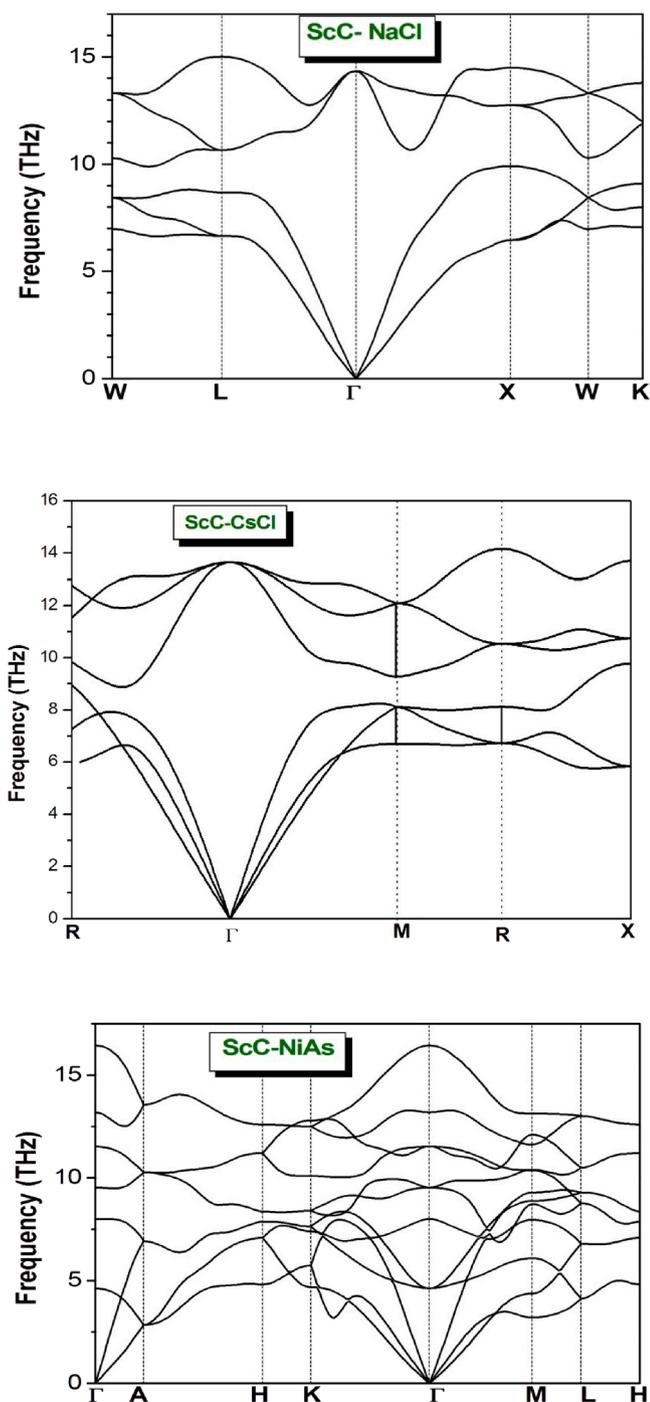


Fig. 4. Calculated phonon dispersion curves of NaCl at 0GPa, NiAs at 27.15 GPa and CsCl at 111 GPa.

rule [38]. If the ratio is lower, the material is considered to be brittle and vice versa. For the two stable structures, NaCl and NiAs, we found NaCl to be brittle and the NiAs to be ductile. The Poisson's ratio also indicates, whether a bonding is ionic, ratio higher or close to 0.25, or if the bonding has covalent character. From the results (Table 6), we determine both structures to be ionic [39,40]. Young's modulus values for the unstable CsCl and ZB structure are negative. On the other hand Young's modulus and Shear's modulus values for NaCl structure are greater than NiAs structure values; this indicates that NaCl structure is more stable than NiAs structure. Shear's modulus values for the unstable CsCl and ZB structure are negative. As a result of high Young's modulus and Shear's modulus values within the NaCl structure; elastic wave

velocity and Debye temperature within NaCl structure are twice their values within NiAs structure. To the best of our knowledge, no results from former works are available, giving any information about Poisson's modulus.

To check the dynamical stability of the NaCl, CsCl, WZ and NiAs polytypes of ScC, we have calculated their phonon dispersion curves along the high symmetry lines of their corresponding Brillouin zone using the linear response approach designed within density functional perturbation theory [41] as implemented in the CASTEP code [42]. As shown in Fig. 4, no imaginary phonon modes are found throughout the Brillouin zone (i.e., all frequencies are positive) in the phonon dispersion diagrams calculated for the NaCl at 0 GPa, NiAs at pressure ranging from zero to 27.15 GPa and CsCl at 111 GPa phases. These results highlight the dynamical stability of ScC in these phases at their corresponding phase transition pressure. However, the phonon dispersion curves WZ and ZB phases as well as CsCl at zero pressure (not presented for brevity) show imaginary phonon modes (i.e., negative frequencies), which suggest the no dynamical stability of ScC in the aforementioned phases.

It should be noted that according to the phonon computation WZ is found to be dynamically unstable, but, according to the mechanical stability criteria it is mechanically stable. In general, if a system is dynamically stable most of the time it is also mechanically stable. If a system is dynamically unstable and mechanically stable, it indicates that this particular phase is a metastable structure.

The solid-state NEB approach has been employed at transition pressure (111GPa) to simulate the pathway transition from NaCl to the CsCl phase. Nine intermediate images were used in this process. The root-mean-square (RMS) force convergence has been fixed at 0.03 eV/Å for each image. The spring constant is within a range of 0.2–1.5 eV/Å².

As shown in Fig. 5, our intermediate sub group (R-3) allows us to find one process with a change of angle from 60 to 90°. The saddle point was found in the middle of the pathway in image number 6. The enthalpy barrier was found to be 70.40 kJ/mol, lower than 100 kJ/mol, which suggests that the martensitic mechanism is possible from NaCl to CsCl along the R-3 pathway.

Electronic properties

The calculated densities of state (DOS) and the band structures for each phase using the PBE-GGA are displayed in Figs. 6–11, respectively.

The calculated band structures of ScC do not show regions of forbidden energy in the CsCl, NaCl, NiAs, WZ and ZB phases as shown in Fig. 11 (a → e). Therefore, one can conclude the whole studied structures have a metallic character.

The DOS as a function of energy, for each phase of ScC compound are displayed in Figs. 6–10. For each of the phases the DOS is plotted for the C-atom as well as for the Sc-atom, together with the total DOS of the compound. The density of states usually used to estimate the number of states available to be occupied for each energy level. The density of states is divided into two regions, valence band; bands below the Fermi energy level; and conduction band. The region just below the Fermi level as seen in Figs. 6–10 is mainly from C-p and Sc-d states, while the far region below the Fermi level is mainly from C-s state. Region above the Fermi level is mainly from Sc-d state with small contribution from C-p and C-s state.

Optical properties

In this section, we are focusing on the optical properties for the ground state phase NaCl of ScC. Using Kramers-Kronig relations, one can calculate the complex dielectric function $\epsilon(\omega)$ which is given by $\epsilon(\omega) = \epsilon_1(\omega) + i\epsilon_2(\omega)$, the real part $\epsilon_1(\omega)$ and the imaginary part $\epsilon_2(\omega)$ of the dielectric function represent the electronic polarizability under incident light and material absorption of light behavior, respectively [43,44]. The acknowledge of the real and imaginary parts of dielectric function $\epsilon(\omega)$ allows us to compute some optical constants such as the optical

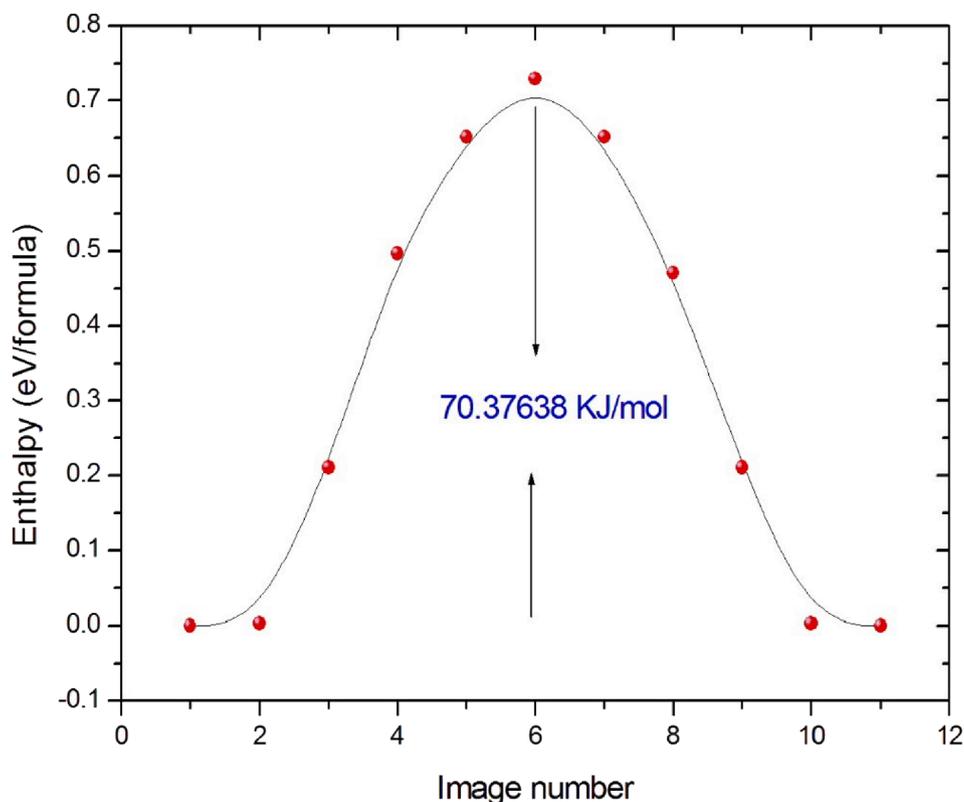


Fig. 5. Enthalpy barrier for ScC: NaCl \rightarrow CsCl transformation at the transition pressure $P_t = 111$ GPa along the "rhombohedral" R-3 path.

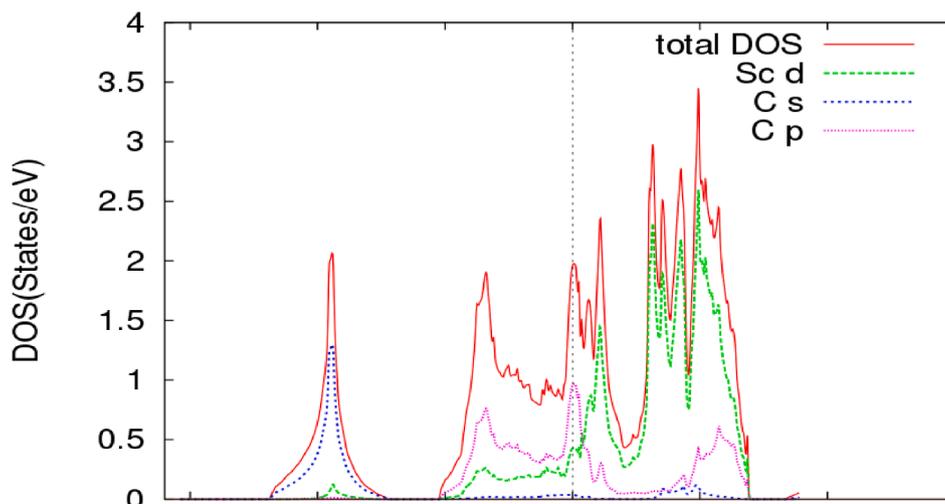


Fig. 6. Density of State of ScC in the CsCl structure.

conductivity $\sigma(\omega)$, refractive index $n(\omega)$, reflectivity $R(\omega)$, absorption $I(\omega)$ coefficients and energy loss function $L(\omega)$ for a photon energies up to 14 eV using equations (49 to 54) in reference [45].

Fig. 12(a) represents the conductivity spectra $\sigma(\omega)$, of ScC as a function of photon energy. The high value of the static conductivity $\sigma(0)$ of the studied compound is in agreement with previous band structure calculations and indicating that ScC in the NaCl structure is metal.

The complex dielectric function is a very important optical constant; it explains the response of the material to the electric field [46]. Fig. 12 (b and c) shows the dielectric function of ScC. The static values of these two constants $\epsilon_1(0)$ and $\epsilon_2(0)$ (very high negative value for $\epsilon_1(0)$ and very high positive value for $\epsilon_2(0)$), reveal the metallic nature for the

compound under consideration. From the $\epsilon_2(\omega)$ spectrum of Fig. 12(b) one can notice that the $\epsilon_2(\omega)$ value becomes zero beyond energy equals 0.352 eV. The absorption is observed at low photon energies (less than 0.352 eV) since the values of $\epsilon_2(\omega)$ are not zero. The compound is getting transparent beyond the value 0.352 eV when the values of $\epsilon_2(\omega)$ are zero.

Fig. 12(c) shows negative values of $\epsilon_1(\omega)$ for the whole range of energy, maximum negative value at 0 eV and goes to a small negative value at about 2 eV; this material will have metallic behavior rather than dielectric. The values of static dielectric constant $\epsilon_1(0)$ and $\epsilon_2(0)$ are -1200 and 32500 , respectively. The high static dielectric constant reveals that this compound is promising material to be used in manufacturing of high value capacitors [46].

The maximum reflectivity $R(\omega)$ occurs (Fig. 12(d)) when the real part

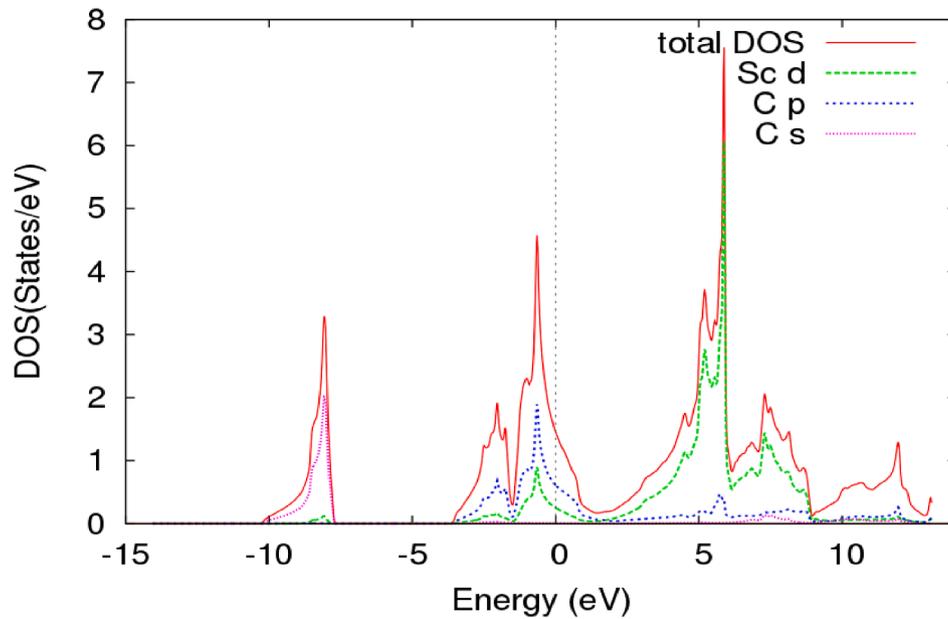


Fig. 7. Density of state of ScC in the NaCl structure.

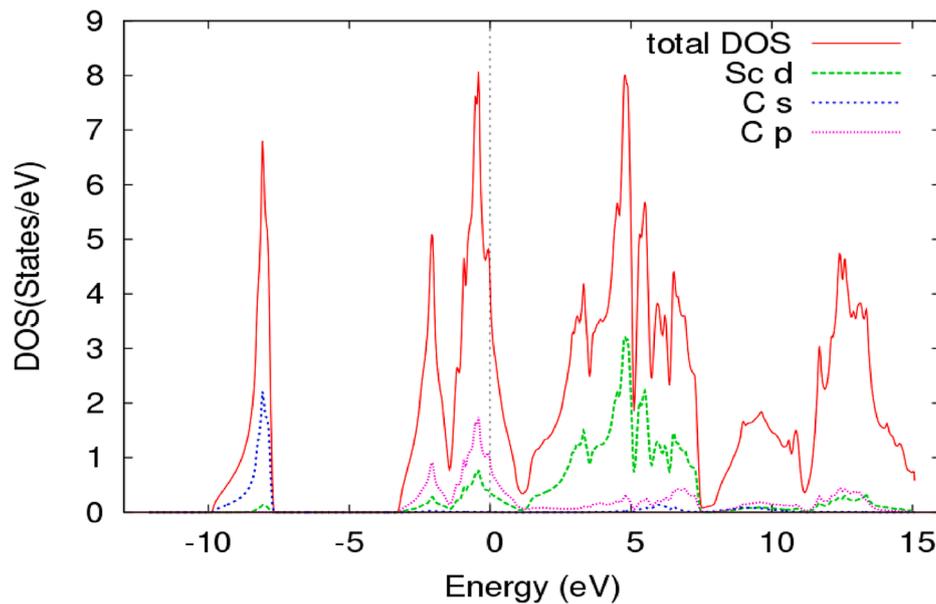


Fig. 8. Density of state of ScC in the NiAs structure.

of dielectric function $\epsilon_1(\omega)$ becomes negative. The static reflectivity $R(0)$ is around 0.98, This value drops rapidly in the low energy region to reach about 0.2 at 3 eV, beyond which $R(\omega)$ begins to rise with well-defined peaks at energies 6 eV and 10 eV as a result of intra-band transition.

The refractive index is an important optical constant which explains how much light is refracted, or bent when light penetrates the material. Fig. 12(e) illustrates the refractive index of ScC compound with large static refractive index $n(0)$ equals to about 91, the refractive index is higher in the low energy region and gradually decreases in this low energy region, it goes to about zero value at 2 eV and has a small values between 3 eV and 9 eV.

Fig. 12(f) shows that the static value of the absorption coefficient $I(0)$ is zero which indicates the metallic behavior of ScC compound in NaCl structure. The high values of the absorption coefficient $I(\omega)$ above 6 eV and the maximum peak appeared in Fig. 12(f) at 9 eV indicate that the

ScC compound is suitable when the absorption is needed in the high energy region. The energy loss function $L(\omega)$ explains the energy loss of a fast electron entering a material. It is shown in Fig. 12(g) as a function of photon energy. Fig. 12(g) shows three main peaks at 3 eV, 12 eV and 13 eV. The highest peak occurs at 12 eV, this peak is coupled to the feature which is associated with plasma resonance, and the corresponding frequency is called bulk plasma frequency [47].

Conclusion

In this work, five different structural phases of ScC compound have been analyzed by investigating the structural, elastic, dynamical, and electronic properties. The calculated structural data are in very good agreement with experimental and theoretical reports. The equation of state indicates, NaCl to be the state with the lowest minimum energy. We conclude that the NaCl-structure is the ground state of ScC

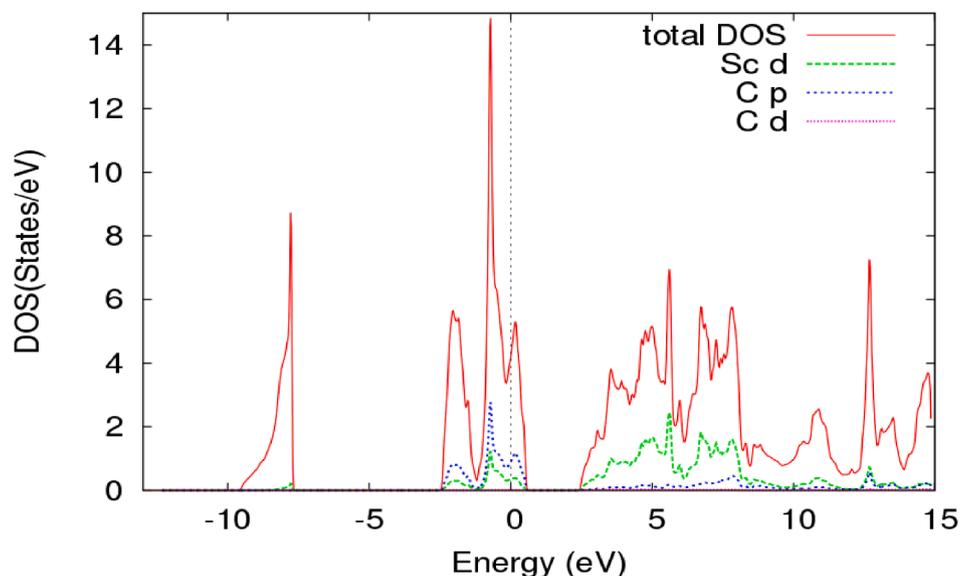


Fig. 9. Density of state of ScC in the WZ structure.

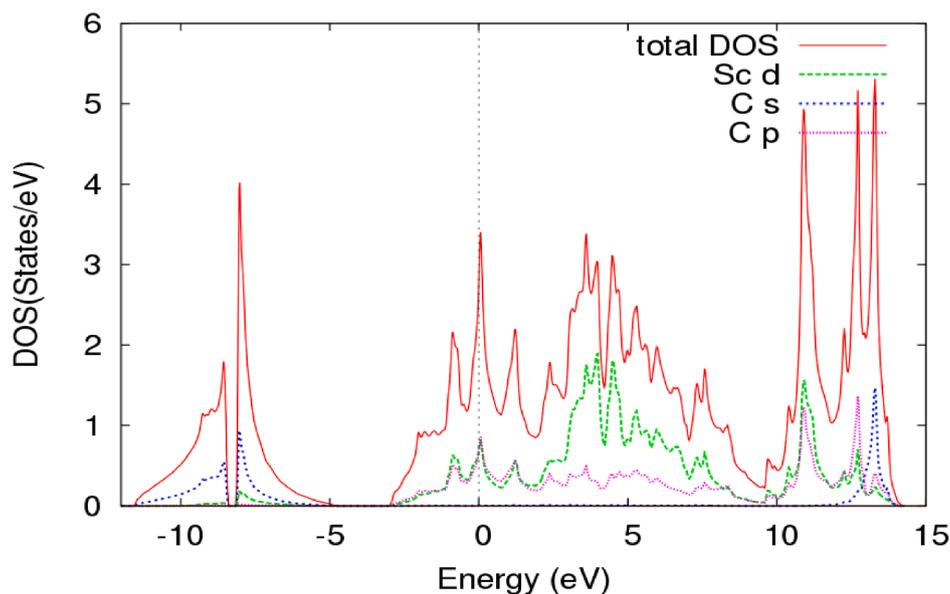


Fig. 10. Density of state of ScC in the ZB structure.

compound among the five studied structures. At ambient conditions, ScC stabilizes in the NaCl structure. By analyzing the elastic properties, we found that NaCl, NiAs and WZ structures are stable. The others are shown to be unstable structures. Optical properties and electronic band structure both indicate that ScC in NaCl structure has a metallic nature. The relative stability of the ScC has been also studied. When external pressure is applied, NaCl transforms into a CsCl at transition pressure of 111 GPa. The phonon calculations reveal that ScC is dynamically stable in the NaCl phase at zero pressure as well as in CsCl and NiAs structures at their corresponding transition pressures. However, the phonon spectra depict imaginary frequencies for both ZB, and WZ structures. The calculated elastic constants indicate that NaCl and NiAs phases are mechanically stable. The WZ structure is found to be a dynamically unstable but mechanically stable phase, which might be a possible indication for a metastable phase. We carefully investigated the mechanism of pressure-induced phase transitions from NaCl to CsCl phases. It is found that the R-3 rhombohedral subgroup needs a reasonable barrier activation energy to allow this energy. One can see from optical

properties calculations that ScC compound in NaCl structure can be used as a good capacitor and also it is an excellent refractive compound.

CRediT authorship contribution statement

Mohammed S. Abu-Jafar: Conceptualization, Methodology, Software, Investigation, Validation, Visualization, Formal analysis, Writing - review & editing, Supervision, Project administration. **Vincent Leonhardt:** Data curation, Methodology, Formal analysis, Writing - original draft, Software, Investigation. **Raed Jaradat:** Data curation, Methodology, Formal analysis, Writing - review & editing, Software, Investigation, Validation. **Ahmad A. Mousa:** Data curation, Methodology, Formal analysis, Writing - review & editing, Software, Investigation, Validation. **Samah Al-Qaisi:** Data curation, Methodology, Formal analysis, Writing - review & editing, Software, Investigation. **Nada T. Mahmoud:** Data curation, Methodology, Formal analysis, Writing - review & editing, Software, Investigation. **Ahmed Bassalat:** Methodology, Formal analysis, Writing - review & editing, Supervision. **R.**

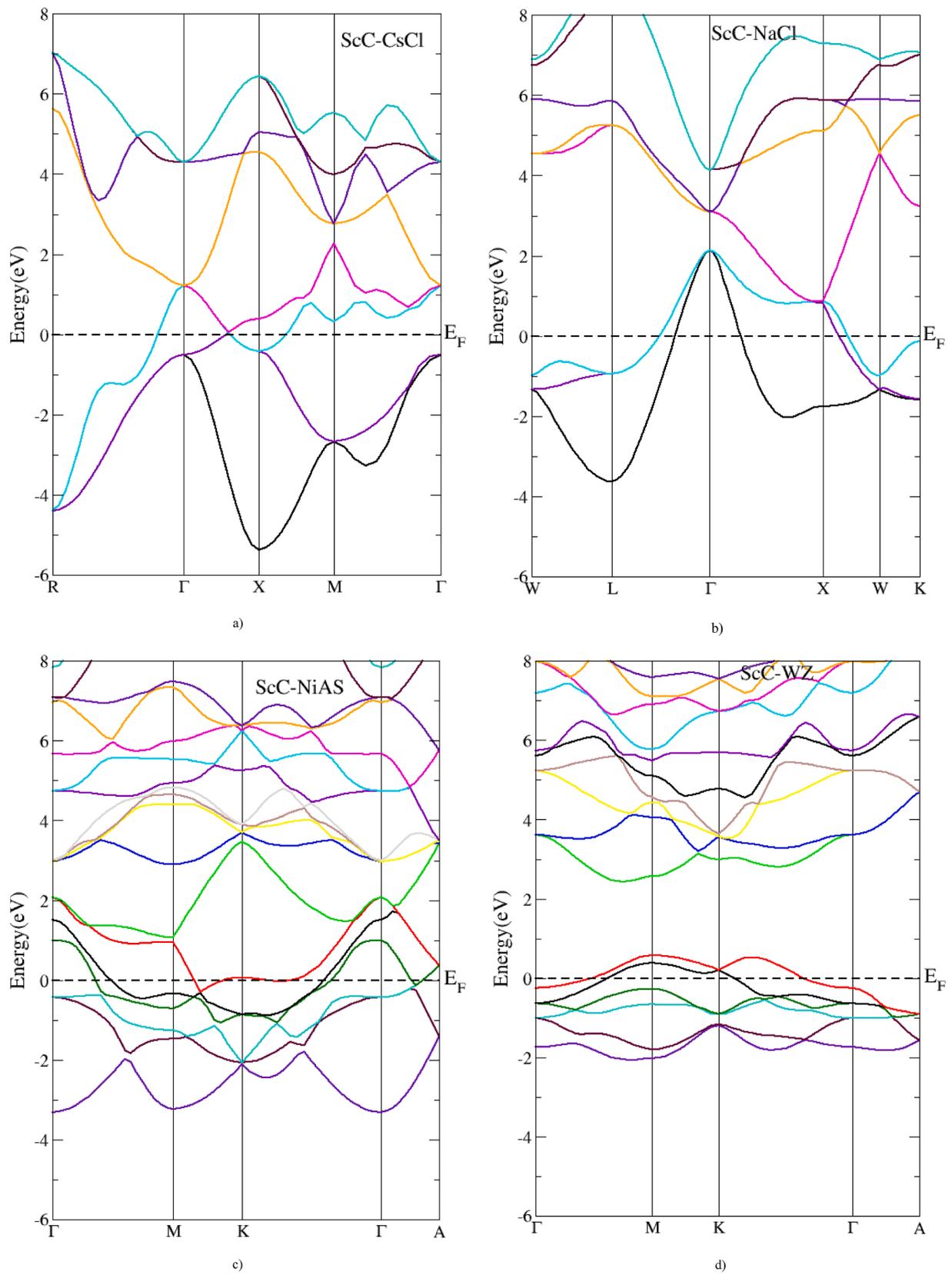


Fig. 11. Band structures of ScC in the a) CsCl b) NaCl c) NiAs d) WZ and e) ZB structures.

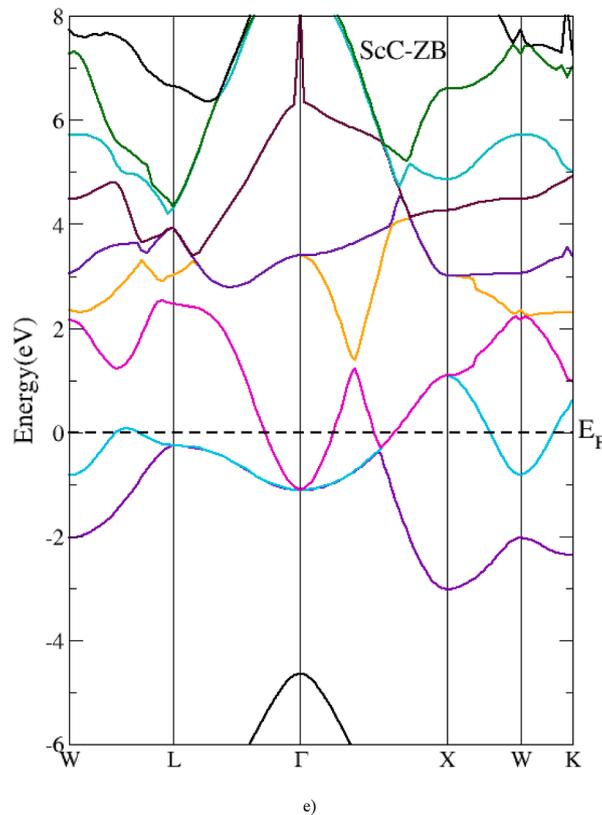


Fig. 11. (continued).

Khenata: Methodology, Formal analysis, Writing - review & editing. **A. Bouhemadou:** Software, Data curation, Formal analysis.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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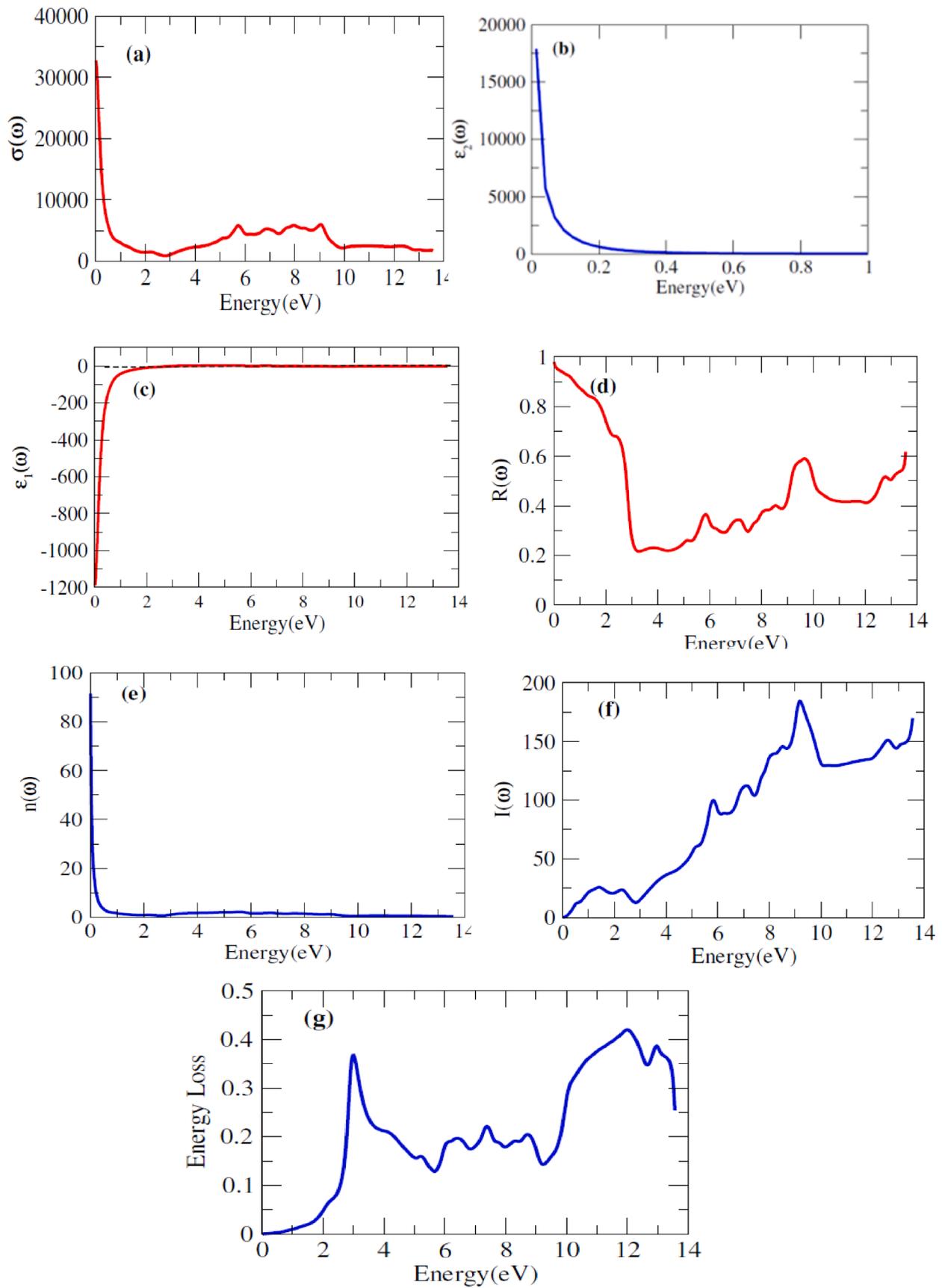


Fig. 12. Optical spectra of ScC in NaCl structure (a) Optical conductivity, (b) Imaginary part of dielectric function $\epsilon_2(\omega)$, (c) Real part of dielectric function $\epsilon_1(\omega)$, (d) Reflectivity $R(\omega)$, (e) Refraction $n(\omega)$, (f) Absorption $I(\omega)$ and (g) Energy loss $L(\omega)$.

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