Structural, elastic, electronic and phonon properties of scandium-based compounds ScX₃ (X = Ir, Pd, Pt and Rh): An *ab initio* study

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ABSTRACT

Self-consistent band calculations on four compounds of the L1₂ structure are presented. The structural, elastic, electronic and phonon properties of ScX₃ (X = Ir, Pd, Pt and Rh) compounds within density functional theory have been investigated. The calculated lattice constants for those compounds are in good agreement with the available theoretical and experimental values. The elastic constants (C_{11}, C_{12} and C_{44}) in L1₂ phase for ScX₃ (X = Ir, Pd, Pt and Pd) compounds are calculated using the energy-strain method. These calculated elastic constants satisfy the mechanical stability criterion and the ductility of ScX₃ (X = Ir, Pd, Pt and Rh) is predicted by Pugh's criterion. The band structure and density of states (DOS), and phonon dispersion curves have been obtained and compared with the available results as well as with existing theoretical calculations. The present band structure calculations predict that the L1₂–ScX₃ (X = Ir, Pd, Pt and Pd) compounds are metals. Finally specific heat at constant volume versus temperature is calculated and discussed using the quasi harmonic approximation.

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1. Introduction

The intermetallic compounds with the formula AB_3 are currently under intense investigations due to their structural and physical properties. These compounds have interesting mechanical properties, those with L1₂ atomic order are significantly more ductile than the compounds which crystallize in D22 phase, they are used for ultra high temperature applications and generally they have high melting points and good corrosion resistance.

Scandium-based compounds ScX₃ (X = Ir, Pd, Pt and Pd) are binary intermetallic compounds with the L1₂ structure, which belongs to Pm-3m space group. The crystal structure of these compounds is displayed in Fig. 1. The structural [1–4], thermo-electrical [5], thermodynamic [6,7], electronic properties [8–14], electronegativity [12], superconductivity [2–4] and phase diagrams [12] of ScX₃ (X = Ir, Pd, Pt and Pd) have been studied by several groups, employing different theoretical and experimental methods. The electronic band structure for IrSc₃ and ScPt₃ compounds in the L1₂ structure has not been studied in detail so far in the available literature. In other hand, electronic properties of L1₂–ScPd₃ have been investigated using first principle calculation based on the full-potential

non-orthogonal local orbital minimum-basis (FPLO) scheme [8], linearized muffin-tin orbital (LMTO) method [12,14] and the linearized augmented plane-wave (LAPW) method [13]. Theoretical and experimental band structure of L1₂–ScRh₃ alloy has been investigated using X-ray photoelectron spectra (XPS), nuclear magnetic resonance spectra (NMR) and *ab initio* calculations (VASP) by Oku et al. [9,11]. In addition, Sahara et al. [10] have also studied the structural and electronic properties of ScRh₃ in the L1₂ structure using the Vienna *ab initio* simulation package (VASP) code within the generalized gradient approximation (GGA). Recently, the elastic constants of L1₂–ScPt₃ have been calculated using of the exact muffin-tin orbitals (EMTO) method [15].

The phonon properties are necessary for a microscopic understanding of the lattice dynamics. The knowledge of the phonon spectrum plays a significant role in determining various material properties such as phase transition, thermodynamic stability, transport and thermal properties. To the best of our knowledge, there are no reports on the study of vibrational properties of these compounds. In an effort to understand them in the present work, first principle calculations are performed to investigate the fundamental properties of ScX₃ (X = Ir, Pd, Pt and Pd) compounds with L1₂ structure including total energy, lattice constant, electronic band structure, density of states, mechanical properties, vibrational properties, and ductility as well.

This paper is organized as follows. Section 2 is devoted to the description of our methods of calculation. We discuss the results

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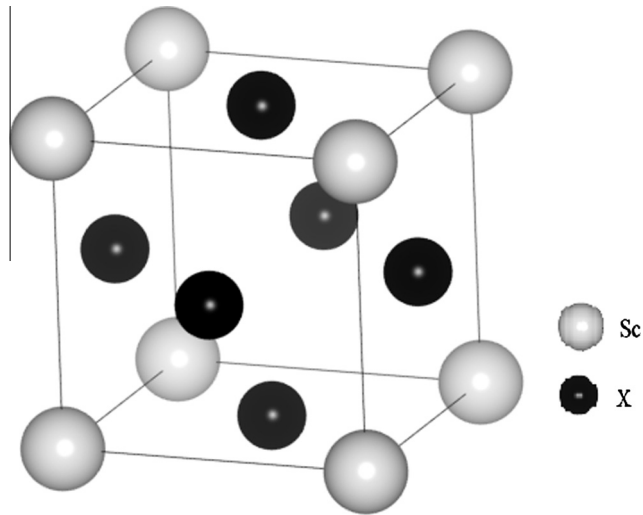*E-mail addresses:* nihat.arikan@hotmail.com (N. Arıkan), charifizoulikha@gmail.com (Z. Charifi).

Fig. 1. Crystal structure of ScX$_3$ (Ir, Pd, Pt and Rh) compounds in the L1$_2$ structure.

of our calculations in Section 3 for the structural, and vibrational properties of ScX$_3$ (X = Ir, Pd, Pt and Rh) compounds, including comparison with experiment. The electronic structure of these compounds is examined. A summary is given in Section 4.

2. Methodology

ScX$_3$ (X = Ir, Pd, Pt and Rh) compounds crystallize in a simple cubic Cu$_3$Au type crystal structure with four atoms per unit cell. It belongs to the P4/nmm space group with Sc occupying the 1a site, and X the 3c sites (see Fig. 1). First-principles studies of the ScX$_3$ (X = Ir, Pd, Pt and Rh) compounds were performed by employing the self-consistent ultrasoft pseudopotential method [16] based on the density functional theory, within the generalized gradient approximation (GGA), incorporated into the quantum-Espresso code [17]. We employed the Perdew–Burke–Ernzerhof (PBE) [18] for the exchange–correlation potential. The wave

functions were expanded in a plane-wave basis set with a kinetic energy cut-off of 40 Ry for L1$_2$ structure. The electronic charge density was evaluated up to the kinetic energy cut-off 400 Ry. Brillouin zone integrations were performed using a $10 \times 10 \times 10$ k-points mesh. Integration up to the Fermi surface was performed using the smearing technique [19] with smearing parameter $\sigma = 0.02$ Ry.

Having obtained self-consistent solutions of Kohn–Sham equations, the lattice-dynamical properties were calculated within the framework of the self-consistent density functional perturbation theory [20,21]. To obtain complete phonon dispersions and density of states, eight dynamical matrices were calculated on a $(4 \times 4 \times 4)$ q-point mesh. The dynamical matrices at arbitrary wave vectors were evaluated using Fourier deconvolution on this mesh. The ground state of each compound was found by minimizing the total energy as a function of the lattice parameter. Specific heats at constant volume versus temperature were calculated using the quasi harmonic approximation (QHA) [22].

The elastic constants can be obtained by calculating the total energy as a function of volume-conserving strains that break the cubic symmetry. The bulk modulus B, C_{44}, and shear modulus $C' = (C_{11} - C_{12})/2$ are calculated from hydrostatic pressure $e = (\delta, \delta, \delta, 0, 0, 0)$, tri-axial shear strain $e = (0,0,0,\delta,\delta,\delta)$ and volume-conserving orthorhombic strain $e = (\delta, \delta, (1 + \delta)^{-2} - 1, 0, 0, 0)$, respectively [23]. Hence, B can be obtained from

$$\frac{\Delta E}{V} = \frac{9}{2}B\delta^2 \tag{1}$$

where V is the volume of unstrained lattice cell, and ΔE is the energy variation as a result of an applied strain with vector $e = (e_1, e_2, e_3, e_4, e_5, e_6)$. C' can be calculated from

$$\frac{\Delta E}{V} = 6C'\delta^2 + 0\delta^3 \tag{2}$$

The two expressions above yield $C_{11} = (3B + 4C')/3$ and $C_{12} = (3B - 2C')/3$, and C_{44} is given by

$$\frac{\Delta E}{V} = \frac{3}{2}C_{44}\delta^2 \tag{3}$$

The details on the calculation of elastic constants have been described in our previous papers [24].

Table 1
Calculated lattice constants (in Å), bulk moduli (in GPa) and pressure derivative of the bulk modulus for ScX$_3$ (X = Ir, Pd, Pt and Rh) compounds in the L1$_2$ structure.

	References	a (Å)	B	B'	C'	C_{11}	C_{12}	C_{44}
ScIr$_3$	This Work	3.958	246.005	3.79	80.64	353.52	192.25	168.53
	Exp. [3]	3.900						
ScPd$_3$	This work	4.015	149.308	3.86	43.53	207.35	120.29	84.42
	Exp. [3]	3.981						
	Exp. [4]	3.909						
	Exp. [8]	3.960						
	Exp. [12]	3.959						
ScPt$_3$	This work	4.024	198.365	3.87	66.14	286.58	154.27	113.91
	Exp. [3]	3.958						
	Exp. [2]	3.958						
	Exp. [4]	3.953						
	LMTO [14]	3.959						
	EMTO-LDA [15]		246.200		78.10	350.30	194.10	72.60
	EMTO-GGA [15]				86.30	379.40	206.90	89.10
	EMTO-LAG [15]				78.30	355.80	199.30	74.30
ScRh$_3$	This work	3.944	190.217	4.62	54.55	262.95	153.85	121.70
	Exp. [3]	3.900						
	Cal. [1]	3.903						
	Exp. [2]	3.898						
	Cal. [4]	3.909						
	VASP [9]	3.860						
	Exp. [9]	3.902						
	Exp. [10]	3.910						
	VASP [10]	3.930						

Table 2
Calculated Debye temperature Θ_D (K), shear modulus G (GPa), B/G, anisotropy factor A, Young's modulus E (GPa), Poisson's ratio σ for ScX_3 (X = Ir, Pd, Pt and Rh) compounds.

	Ref.	B	θ_D	G	B/G	A	E	σ
$ScIr_3$	This Work	263.400	411.380	133.373	1.844	2.090	338.878	0.270
$ScPd_3$	This Work	164.200	348.660	68.063	2.194	1.939	177.255	0.302
$ScPt_3$	This work	221.200	398.700	94.798	2.092	1.722	245.317	0.294
	LDA [15]	246.200	–	74.700	3.330	0.930	203.600	0.360
$ScRh_3$	This work	159.600	388.380	94.836	2.005747	2.230991	243.964	0.286
	VASP [10]	188.700	–	–	–	–	–	–

In general hardness is known to be a material parameter that indicates resistance to elastic or plastic deformation, this parameter is the bulk modulus B or the shear modulus G.

The shear modulus G of a cubic structure is given by:

$$G = \frac{C_{11} - C_{12} + 3C_{44}}{5} \qquad (4)$$

The anisotropy factor A is given by:

$$A = \frac{2C_{44}}{(C_{11} - C_{12})} \qquad (5)$$

As A approaches unity the crystal becomes isotropic. We also list some auxiliary quantities which are often quoted in the literature. The young's modulus for an isotropic solid is related to B and G by the formula:

$$E = \frac{9BG}{3B + G} \qquad (6)$$

Poisson's ratio is also of interest

$$\sigma = \frac{1}{3}\left(1 - \frac{E}{3B}\right) \qquad (7)$$

3. Results and discussion

3.1. Ground-state properties and mechanical stability

The study of the Scandium-based compounds ScX_3 (X = Ir, Pd, Pt and Rh) is an interesting initial step to understand the physical properties of intermetallic compounds with heavier rare earth elements. It has been found that the ScX_3 (X = Ir, Pd, Pt and Rh) compounds were stable in $L1_2$ non-magnetic phase [1,3,8]. The total energy as a function of unit-cell volume around the equilibrium cell volume V_0 for ScX_3 (X = Ir, Pd, Pt and Rh) compounds is calculated for $L1_2$ phase. We determined a set of total energies $E_i = E(V_i)$, and used several volumes which are within 10-30 of the expected equilibrium volume. Then the calculated total energies are fitted to Murnaghan's equation of state [25] to obtain the ground-state properties such as the lattice constants, and the bulk modulus B. The calculated structural parameters of ScX_3 (X = Ir, Pd, Pt and Rh) compounds are listed in Table 1, compared with the available experimental data and other theoretical results [1–4,8–10,14,15]. Our calculated lattice constants agree well with the experimental and other calculations. For $ScPt_3$, our estimation of bulk modulus of 198.365 GPa is smaller than the calculated value using EMTO method (246.2 GPa) [15]. The bulk modulus in these compounds increases with a decrease in the lattice parameter.

Numbers that quantify the response of a particular material to elastic or non-elastic deformation when a stress load is applied to that material are known as Elastic Constants. A knowledge of the elastic constants is important for a variety of reasons. At the most fundamental level the adiabatic elastic constants are given by the second derivatives of the internal energy with respect to strain and thus are related to interatomic potentials. They are also related to the thermal properties of a solid through the Debye

theory. There are several ways of calculating elastic constants. The traditional method is to apply a tension on the sample and calculate the corresponding strain and elastic constants from the tension-strain relationship. To obtain the elastic constants of these
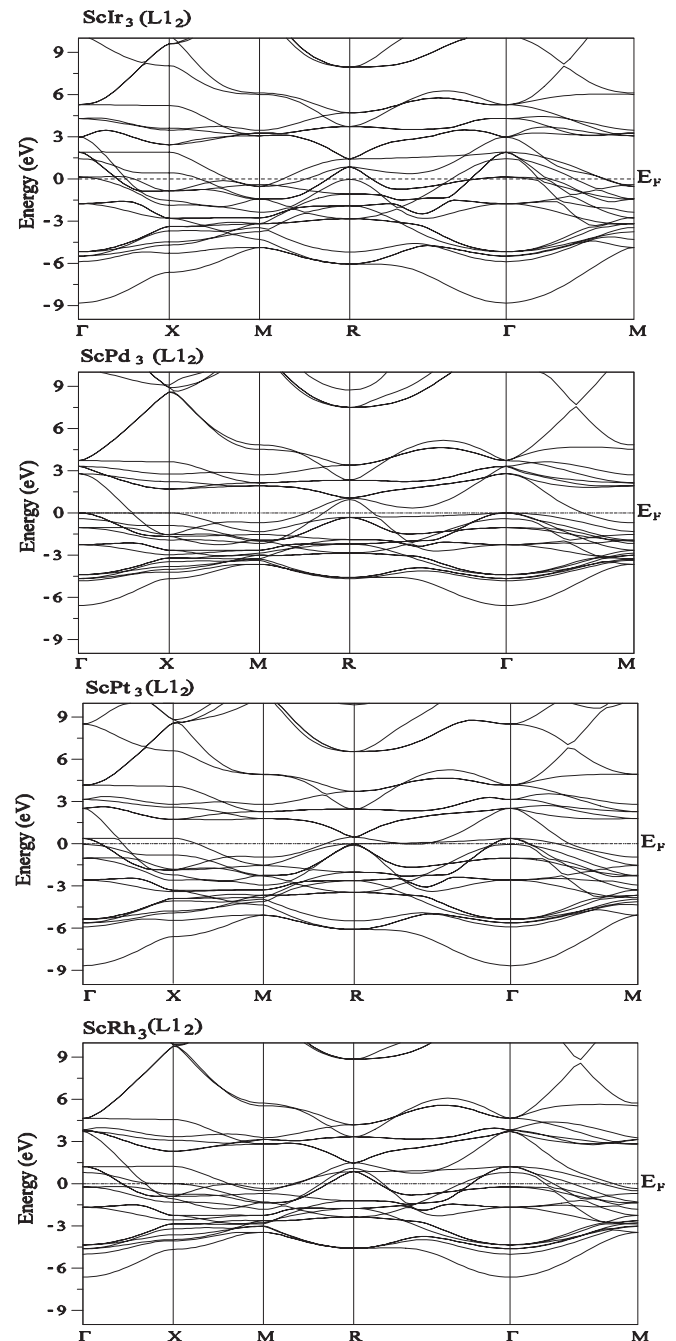
Fig. 2. The electronic band structure for ScX_3 (X = Ir, Pd, Pt and Rh) compounds along several lines of high symmetry in the Brillouin zone.

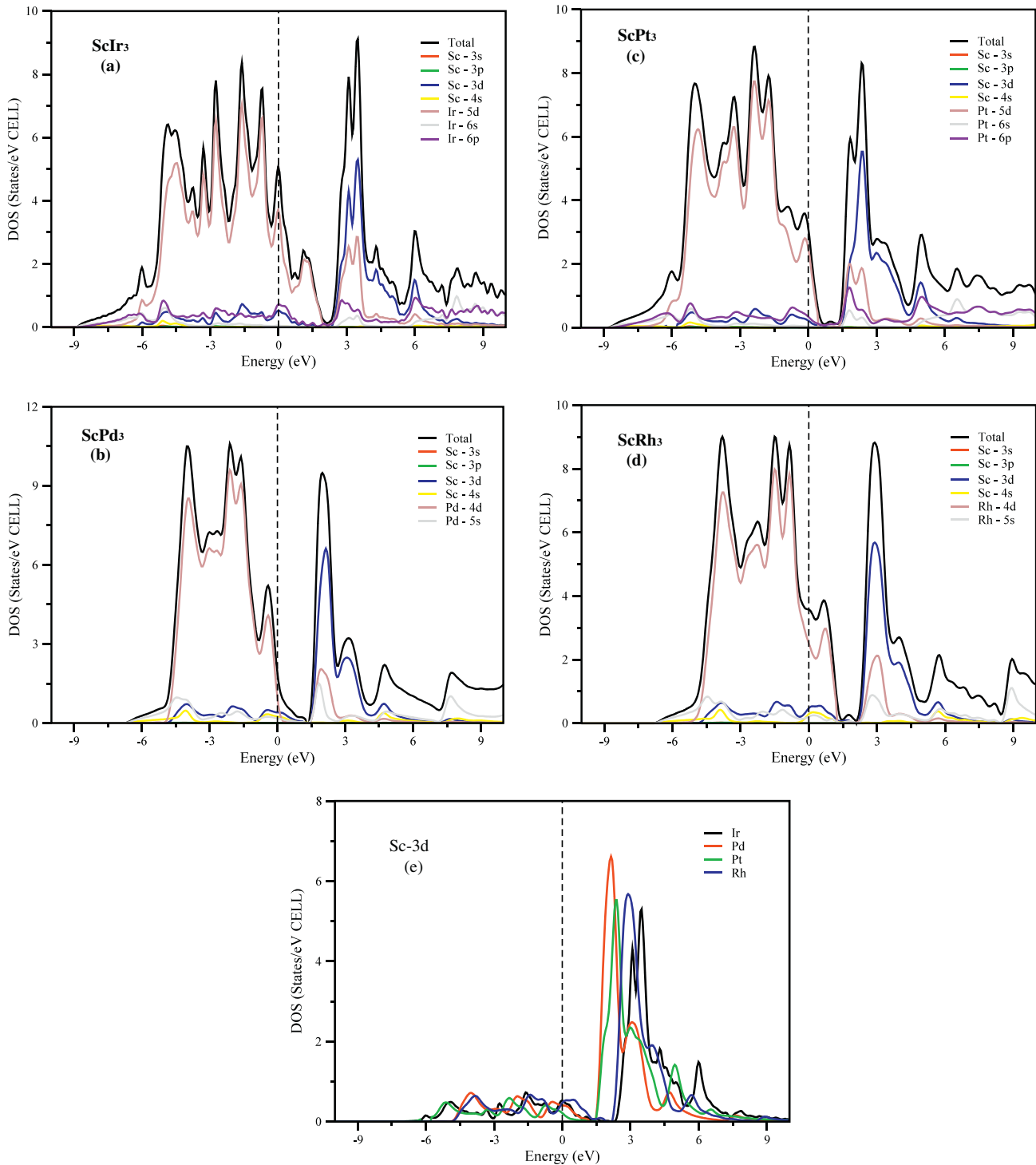**Fig. 3.** Calculated total and partial density of states for ScX$_3$ (X = Ir, Pd, Pt and Rh) compounds.

compounds with cubic structure we have used numerical first principles calculation by computing the components of the stress tensor e for small strains, using the method reported in Ref. [23]. The calculated elastic constants of ScX$_3$ (X = Ir, Pd, Pt and Rh) compounds are listed in Table 1, together with data available from other calculations for comparison [15]. To the best of our knowledge, no experimental values for the elastic constants of these compounds have been appeared in the literature, so our results for L1$_2$ phase can serve as a prediction for future investigations. Our calculated values of C', C_{11}, C_{12} and C_{44} for ScPt$_3$ have been

found to be smaller than those of Ref. [15] by about 18%, 22%, 26% and, 36%, respectively. Mechanical stability of these compounds has been analyzed in terms of their elastic constants. The conditions for mechanical stability for cubic crystals [26] are given by

$$C_{44} > 0, (C_{11} - C_{12})/2 > 0 \text{ and } B = (C_{11} + 2C_{12})/3 > 0. \tag{8}$$

It is clearly seen from Table 1, that these criteria are verified, so we conclude that all the compounds are stable in the L1$_2$ phase.

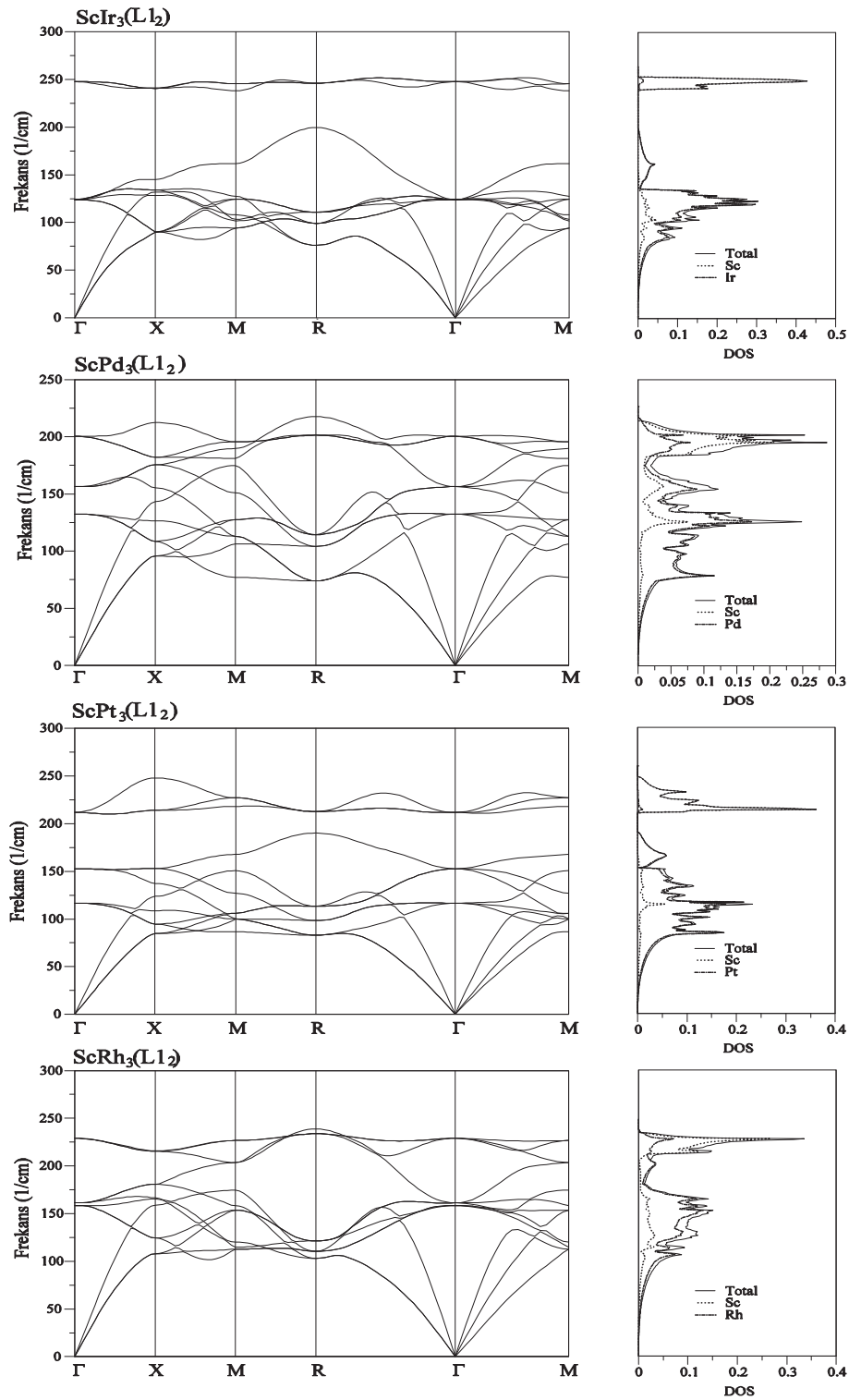**Fig. 4.** Phonon dispersion curves and phonon density of states for ScX_3 (X = Ir, Pd, Pt and Rh) compounds along several lines of high symmetry in the Brillouin zone.

In order to investigate the mechanical properties of ScX_3 (X = Ir, Pd, Pt and Rh) compounds, brittleness and ductility properties have also been studied by using the bulk modulus to shear modulus B/G ratio and Poisson's ratio σ. According to Pugh [27], B/G ratio is greater than 1.75, so all the compounds are ductile. This is in good agreement with the results found for $ScPt_3$ [15]. It is clearly seen that Poisson's ratios of our compounds are around 1/3, so all of them are ductile. On the basis of the Poisson's ratio shown in Table 2, the brittleness and ductility prop-

erties of ScX_3 (X = Ir, Pd, Pt and Rh) found are in good agreement with the results estimated by the B/G ratio. The Young's modulus of a material is the usual property used to characterize stiffness. The higher the value of E, the stiffer the material is. The largest Young's modulus among the compounds in Table 2 is that of $ScIr_3$, so we conclude that the $ScIr_3$ is the stiffest one. The anisotropy factor A, which is a measure of the degree of elastic anisotropy in the crystal, is calculated and its values is found to be far from 1 (see Table 2), so we conclude

that the compounds under consideration in this work are strongly anisotropic elastically.

3.2. Electronic and vibrational properties

The calculated electronic band structure of ScX_3 (X = Ir, Pd, Pt and Rh) compounds along the higher symmetry directions Γ, X, M and R in the Brillouin zone using (GGA) approach are calculated and given in Fig. 2. It is seen that there is no band gap at the Fermi level, as a result, ScX_3 (X = Ir, Pd, Pt and Rh) compounds exhibit a metallic behavior. The Fermi level E_F is shown by a broken horizontal line which intersects the $E(k)$ curves. Our calculated electronic band structure for $ScPd_3$ and $ScRh_3$ are in good agreement with previous reported works [8–14].

In the band structure of ScX_3 (X = Ir, Pd, Pt and Rh) compounds, the main contribution to the total DOS comes from the d orbitals of Ir, Pd, Pt and Rh. The 3d orbitals of Sc hybridize with those of Ir, Pd, Pt and Rh and contribute also significantly to the DOS, but most of the occupied states are the Ir, Pd, Pt and Rh d states. From the total and the partial density of states of ScX_3 (X = Ir, Pd, Pt and Rh) compounds shown in Fig. 3, we note that there are two peaks below and above the Fermi level. The first one is from the Ir, Pd, Pt and Rh 4d states and the second one is due to both Sc 3d and Ir, Pd, Pt and Rh 4d states. Above the Fermi level there is a broad minimum in the density of states looks as a "pseudogap" especially for the $ScPd_3$. This is an indication that $ScPd_3$ is the more stable in the $L1_2$ phase. Traditionally the stability in compounds is associated with low density of states (DOS) at the Fermi energy E_F [28]. For this purpose we have calculated the density of states at the Fermi level $N(E_F)$. The value of this parameter is 1.90, 3.11, 3.58 and 5.06 states/eV Cell for $ScPd_3$, $ScPt_3$, $ScRh_3$ and $ScIr_3$, respectively. We conclude that the $ScPd_3$ has the lowest $N(E_F)$, this confirms that $ScPd_3$ is the more stable compound. Also from Fig. 3e, one can notice that Sc 3d states in ScX_3 (X = Ir, Pd, Pt and Rh) compounds shift to higher energies in the following sequence from $ScPd_3$ to $ScPt_3$ to $ScRh_3$ and $ScIr_3$.

In Fig. 4, we have plotted the phonon dispersion curves, total and partial density of states (DOS) of ScX_3 (X = Ir, Pd, Pt and Rh) compounds in the $L1_2$ structure. The phonon properties of ScX_3 (X = Ir, Pd, Pt and Rh) compounds are calculated within the generalized gradient approximation in the $L1_2$ (Cu$_3$Au) structure, with space group symmetry Pm-3m (221). There are four atoms in the unit cell so the phonon dispersion relation will reveal three acoustic branches and nine optical branches. In our previous paper, we have reported that the phonon branches reduce some symmetry directions [29]. Due to the symmetry, the distinct number of branches is reduced along the principal symmetry directions Γ–X and M–R–Γ in the $L1_2$ structure. For $ScIr_3$ and $ScPt_3$, the highest optical branches are separated from the rest of the phonon branches. This gap is calculated to be around 19.61 cm^{-1} and 41.73 cm^{-1}, respectively. For total DOS of ScX_3 (X = Ir, Pd, Pt and Rh) compounds, the highest frequency of these compounds are located at 249.90 cm^{-1}, 193.30 cm^{-1}, 213.82 cm^{-1} and 224.61 cm^{-1}, respectively. From the partial DOS, it can be inferred that the vibrational mode are mostly excited by Sc atom in the high frequencies, however Ir (Pd, Pt and Rh) atoms contribute a major part to the modes with lower frequencies. The frequencies of the optical phonon modes of ScX_3 (X = Ir, Pd, Pt and Rh) are calculated and found to be 122.78 and 246.37 cm^{-1} for $ScIr_3$, 132.58, 156.51 and 200.98 cm^{-1} for $ScPd_3$, 116.38, 153.5 and 211.62 cm^{-1} for $ScPt_3$, and 158.4, 161.2 and 229.13 cm^{-1} for $ScRh_3$. The calculated phonon dispersion curves of ScX_3 (X = Ir, Pd, Pt and Rh) show that all compounds are dynamically stable in the $L1_2$ structure without any imaginary phonon frequencies. Unfortunately the experimental or theoretical phonon frequencies of ScX_3 (X = Ir, Pd, Pt and Rh) compounds are not available in the literature for further

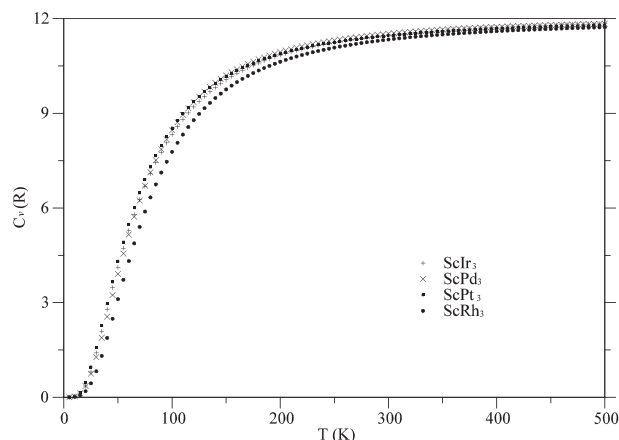**Fig. 5.** The specific heats at constant pressure versus temperature for ScX_3 (X = Ir, Pd, Pt and Rh) compounds.

comparison. Our phonon calculations are in good agreement with our earlier work [30] which belong to the same space group and structure. Fig. 5 shows the calculated specific heat capacity at constant volume (C_v) of ScX_3 (X = Ir, Pd, Pt and Rh) compounds as a function of temperature. The C_v increases rapidly in the range 0–300 K before it starts to saturate. The calculated specific heat capacity C_v is very close to the Dulong-Petit limit [31] at high temperature, which is commonly satisfied with all solids at high temperatures. For all materials, the C_v functions flatten out as the temperature increases above 300 K. The optic and acoustic modes have large effects on the heat capacity.

4. Conclusions

The structural, elastic, electronic and phonon properties of states of ScX_3 (X = Ir, Pd, Pt and Rh) compounds have been studied. Pseudopotential method was used in the framework of the density functional theory (DFT) with the generalized gradient approximation (GGA). The lattice constants and bulk moduli are determined and are in excellent agreement with the available experimental data and theoretical values. We have also studied the mechanical properties of these compounds. The elastic constants have been calculated using the approach, the energy-strain method. The values obtained for $ScPt_3$ are in reasonable agreement with those obtained previously. The calculated elastic constants satisfy the mechanical stability criterion and the ductility of ScX_3 (X = Ir, Pd, Pt and Rh) is predicted by Pugh's criterion. In addition to that the ductility properties of ScX_3 (X = Ir, Pd, Pt and Rh) determined by Poisson's ratio σ criterion are in good agreement with the results estimated by the B/G ratio. The band structure and densities of states DOS for the four alloys are analyzed and compared. They showed that all materials exhibit metallic character. We have also calculated the phonon frequencies along the high symmetry directions. The calculated phonon dispersion curves of ScX_3 (X = Ir, Pd, Pt and Rh) confirm that four compounds are dynamically stable in the $L1_2$ structure without any imaginary phonon frequencies. Finally, using the calculated phonon density of states, the specific heats at constant volume versus temperature have been determined with the quasi harmonic approximation. We conclude that the $ScPt_3$ and $ScPd_3$ alloys could be used as materials for ultra high temperature applications, where the ductility offered by $ScPt_3$ and $ScPd_3$ alloys is an advantage in comparison with that of $ScIr_3$.

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