Research Article

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Elastic properties and plane acoustic velocity of cubic $\text{Sr}_2\text{CaMoO}_6$ and Sr_2CaWO_6 from first-principles calculations

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Abstract: The elastic properties and plane acoustic velocity of double perovskite $\text{Sr}_2\text{CaMoO}_6$ and Sr_2CaWO_6 are investigated with the plane wave pseudopotential method based on the first-principles density functional theory within the local density approximate (LDA) and the generalized gradient approximation (GGA). The calculations indicate that $\text{Sr}_2\text{CaMoO}_6$ and Sr_2CaWO_6 respectively have the the Mo-O and W-O stable octahedral structure. The bulk modulus B , shear modulus G , Young's modulus E , Poisson's ratio ν and Debye temperature were calculated based on the elastic constants. The three dimensional plane acoustic velocities and their projection are in calculated for each direction by solving the Christoffel's equation systematically based on the theory of acoustic waves in anisotropic solids, the result shows of anisotropy of lattice vibration for $\text{Sr}_2\text{CaMoO}_6$ is stronger than Sr_2CaWO_6 .

Keywords: $\text{Sr}_2\text{CaMoO}_6$; Sr_2CaWO_6 ; elastic properties; plane acoustic velocities; the first principles

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1 Introduction

The synthesis and physical properties of $\text{A}_2\text{BB}'\text{O}_6$ -type double perovskites have been widely investigated [1–4] because of their promising applications in optoelectronics or spintronics areas. The ideal double perovskites belong to the cubic space group $Fm\bar{3}m$, in which the crystallization site A is occupied by alkaline earth metal or rare earth

metal element, and the crystallization sites B and B' are often occupied by transition or lanthanide elements [2]. However, for some $\text{A}_2\text{BB}'\text{O}_6$ -type double perovskites, the crystallization sites B and B' can be occupied by one transition metal and another element, such as Ca, Mg, Ln, Sb, Mo or W [4]. In $\text{A}_2\text{BB}'\text{O}_6$ -type double perovskites, the charge and size of cation B differ greatly from those of cation B', and consequently the octahedral units BO_6 and $\text{B}'\text{O}_6$ play dominating roles in their chemical and physical properties [1–4].

Hank *et al.* [5] synthesized $\text{Sr}_2\text{CaMoO}_6$ and Sr_2CaWO_6 through a solid-state reaction and stated that $\text{Sr}_2\text{CaMoO}_6$ and Sr_2CaWO_6 were also two important $\text{A}_2\text{BB}'\text{O}_6$ -type double perovskites with the crystallization site B occupied by the alkaline earth metal Ca and the crystallization site B' occupied by the transition element Mo(W). Both $\text{Sr}_2\text{CaMoO}_6$ and Sr_2CaWO_6 are direct-gap semiconductors, and their experimental band gaps are respectively 2.9 and 3.8 eV. Zhao *et al.* [6] calculated the electronic structures and optical properties of the B-site ordered double perovskites Sr_2MMoO_6 ($M = \text{Mg, Ca or Zn}$) using density functional theory (DFT), and they pointed out that $\text{Sr}_2\text{MgMoO}_6$ and $\text{Sr}_2\text{CaMoO}_6$ exhibit direct band gaps, while $\text{Sr}_2\text{ZnMoO}_6$ has an indirect band gap. The study [6] also revealed that the replacement of the B-site element in double perovskites is a potential method of altering the electronic structure to absorb visible light, and this method could lead to the development of inorganic perovskite solar cells.

The plane acoustic velocity and elastic properties have not been investigated in the previous works for $\text{Sr}_2\text{CaMoO}_6$ and Sr_2CaWO_6 , namely cubic structure. In this work we discussed the elastic modulus, and elastic properties of double perovskite $\text{Sr}_2\text{CaMoO}_6$ and Sr_2CaWO_6 . All research provides a useful theoretical basis for their scientific and technological applications of the $\text{Sr}_2\text{CaMoO}_6$ and Sr_2CaWO_6 crystals.

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2 Calculation method

The elastic properties and plane acoustic velocity of $\text{Sr}_2\text{CaMoO}_6$ and Sr_2CaWO_6 were calculated by the first-principles plane wave pseudopotential method within density functional theory coded in the CASTEP software package [7]. Exchange correlation energy was described by the Perdew-Burke-Ernzerhof parameterization within the generalized gradient approximation (GGA-PBE) [8]. The local density approximation / Ceperley-Alder exchange-correlation potential parameterized by Perdew and Zunger (LDA - CAPZ) [9] was used as a comparative study in geometric optimization. The ultrasoft pseudopotentials were used to describe the interactions between valence electrons and the ionic core, and the typical valence electron configurations considered in the current work included $\text{Sr}:4s^24p^65s^2$, $\text{Ca}:3s^23p^64s^2$, $\text{Mo}:4s^24p^64d^55s^1$, $\text{W}:5s^25p^65d^46s^2$ and $\text{O}:2s^2p^4$, respectively.

The cut-off energy of the plane-wave basis was 500 eV for both $\text{Sr}_2\text{CaMoO}_6$ and Sr_2CaWO_6 after convergence tests. Integrations in the Brillouin zone were carried out on a Monkhorst-pack k-point [10] mesh with spacing of 0.04 nm^{-1} for all calculations. The Broyden-Fletcher-Goldfarb-Shanno (BFGS) quasi-Newtonian minimization method [11, 12] was used in the structure optimization of $\text{Sr}_2\text{CaMoO}_6$ and Sr_2CaWO_6 , and their stable crystal structures could be obtained until the change in total energy was less than $5.0 \times 10^{-6} \text{ eV}$, the maximum ionic Hellmann-Feynman force was converged to $0.01 \text{ eV/\AA}$, the maximum stress tensor was reduced to 0.02 GPa , and the displacement deviation was smaller than $5.0 \times 10^{-4} \text{ \AA}$. The elastic properties and plane acoustic velocity of $\text{Sr}_2\text{CaMoO}_6$ and Sr_2CaWO_6 were further studied based on the obtained stable crystal structures after fully relaxation.

3 Results and analysis

Figure 1 displays the cubic crystal structures of double perovskites $\text{Sr}_2\text{CaMoO}_6$ and Sr_2CaWO_6 with the space group $Fm\bar{3}m$ (No.225), in which Sr atoms occupy the 8c positions, Ca atoms occupy the 4b positions, W (Mo) atoms occupy the 4a positions, and O atoms occupy the 24e positions, respectively.

Table 1 shows the calculated and experimental lattice parameters and cell volumes of $\text{Sr}_2\text{CaMoO}_6$ and Sr_2CaWO_6 . Compared with those calculated by LDA-CAPZ, the lattice parameters and cell volumes obtained from GGA-PBE agree well with the experimental values. Thus,

the GGA-PBE method was adopted in the following calculations.

After geometric optimization, the plane wave pseudopotential approach with GGA-PBE was used to calcu-

Figure 1: The crystal structure of $\text{Sr}_2\text{CaMoO}_6$ or Sr_2CaWO_6

Table 1: Lattice constant $a/\text{\AA}$, density $\rho/\text{g cm}^3$, elastic constant C_{ij}/GPa , Bulk modulus (B), shear modulus (G), and Poisson ratio (σ), V_l (longitudinal), V_s (shear) and V_m (mean) in m/sec , and Debye temperature (θ_D).

Material	$\text{Sr}_2\text{CaMoO}_6$		Sr_2CaWO_6	
Method	LDA	GGA	LDA	GGA
a	8.135293	8.317116	8.151813	8.33765
Exp	8.281		8.308	
ρ	5.02406	4.70172	6.07150	5.67467
V	538.4	576.0	545.9	579.6
C_{11}	292.6	236.1	302.7	246.4
C_{12}	65.0	55.8	63.9	56.7
C_{44}	54.0	37.2	57.4	55.2
B	140.9	115.8	143.5	119.9
G	73.2	53.5	77.3	68.7
E	187.19	139.1	196.6	173.0
σ	0.278584	0.299825	0.271662	0.259454
B/G	1.9248	2.1644	1.8564	1.7452
A^E	0.50021	0.532428	0.505503	0.414749
A^Z	0.475561	0.412646	0.480703	0.581972
V_l	3817.05	3373.25	3690.79	3479.43
V_t	6889.96	6308.81	6591.69	6104.99
V_m	4252.19	3767.76	4108.07	3867.14
θ_D	548.89	506.93	588.48	553.97

Figure 2: Plane acoustic velocities of $\text{Sr}_2\text{CaMoO}_6$ and Sr_2CaWO_6 3D projected images (From left to right is the two transverse velocities and a longitudinal wave, respectively) (GGA)

late the energy band structures and density of states of $\text{Sr}_2\text{CaMoO}_6$ and Sr_2CaWO_6 in the first Brillouin zone. As shown in Figure 2(a), the calculated band gaps of $\text{Sr}_2\text{CaMoO}_6$ and Sr_2CaWO_6 were respectively 2.02 eV and 2.782 eV, smaller than the experimental ones obtained by Hank, i.e. 2.9 eV and 3.8 eV [5]. It should be pointed out that the current calculated band gap of $\text{Sr}_2\text{CaMoO}_6$ is close to that of Zhao [6]. Although the GGA exchange correlation function usually underestimates the band gaps of materials, primarily owing to the discontinuity of exchange-correlation energy, this does not influence the electronic structure analysis [13].

3.1 Elastic properties

Table 1 lists the lattice constants and elastic constants which have been calculated using the LDA and GGA approximations. The LDA approximation underestimates lattice constants, while overestimates the elastic constants. After analysis, the calculated lattice constants are close to

the experimental value. To our best knowledge, no published experimental or theoretical data exist on relevant elastic constants for $\text{Sr}_2\text{CaMoO}_6$ and Sr_2CaWO_6 . The traditional mechanical stability conditional in the cubic crystals are judged by the elastic constants:

$$\begin{aligned} C_{11} > 0, C_{44} > 0, C_{11} > |C_{12}|, \\ C_{11} + 2C_{12}, C_{11} + C_{12} > 0. \end{aligned} \quad (1)$$

For $\text{Sr}_2\text{CaMoO}_6$ and Sr_2CaWO_6 is the calculated elastic constants (C_{ij}) in Table 1 satisfy these Eqs. (1), indicating that they are mechanically stable.

Based on elastic constants, Voigt and Reuss approximations [14] are widely used to calculate the bulk modulus B and the shear modulus G of solids. The bulk modulus B reflects the ability of solids to defend compression, while the shear modulus G stands for the ability of solids to defend shear deformation. For a cubic system, the Voigt and Reuss approximations of B and G can be obtained by:

$$B_V = B_R = \frac{1}{3} (C_{11} + 2C_{12}) \quad (2)$$

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

$$G_V = \frac{1}{5}(C_{11} - C_{12} + C_{44}) \quad (4)$$

$$B = (B_R + B_V)/2 \quad (5)$$

$$G = (G_R + G_V)/2 \quad (6)$$

Hill [15] confirmed that the Voigt and Reuss models represent the extreme upper and lower bounds, respectively, and the arithmetic average value VRH (Voigt-Reuss-Hill) is close to experimental results. The bulk modulus B shear modulus G , results can be determined using the Voigt-Reuss-Hill averaging scheme based on the calculated elastic constants. They can be respectively represented by Eq. (5) and Eq. (6) [16–20].

The calculated bulk modulus B and shear modulus G of ZBO are summarized in Table 1. It can be noted that the bulk modulus B obtained from Eq. (5) matches well with that obtained from the Birch-Murnaghan Equation of State at zero pressure, indicating that our calculation is self-affirming and reliable.

Based on Eqs. (5) and (6), Young's modulus E , Poisson's ratio γ and anisotropic index A^U are determined by:

$$E = 9BG/(3B + G) \quad (7)$$

$$\gamma = \frac{3B - 2G}{2(3B + G)} \quad (8)$$

$$A^U = 5 \frac{G_V}{G_R} + \frac{B_V}{B_R} - 6 \quad (9)$$

The mechanical properties of semiconductor materials, such as the ductility and brittleness, are of high importance for their applications. The calculated young's modulus E and Poisson's ratio σ of uniaxial stress on the uniaxial is defined as the ratio of Hook's law [21–24]. When the value of Young's modulus is high, the material is stiff. The calculated Young's modulus indicates Sr_2CaWO_6 is stiffer than $\text{Sr}_2\text{CaMoO}_6$ with in both LDA and GGA approximations. Based on elastic coefficients, Pugh proposed a criterion for judging the ductility or brittleness of materials: when $B_H/G_H > 1.75$, the material behaves in ductile manner, otherwise it has brittle nature. As shown in Table 1, the values of B_H/G_H ratio are always larger than the critical value, displaying that both compounds are ductile in nature. Both the value of the B_H/G_H ratio and Poisson's ratio of $\text{Sr}_2\text{CaMoO}_6$ are higher than that of Sr_2CaWO_6 , meaning

that $\text{Sr}_2\text{CaMoO}_6$ have a better toughness of the material. The values of Poisson's ratio ν tell us about the characteristics of the bonding forces. In solids, the lower and upper limits for the central forces respectively are 0.25 and 0.5. For both semiconductors, the obtained values of ν are in the range of 0.25–0.5, indicating that the interatomic forces are ruled by central forces and there exist ionic character in the bonding.

The elastic anisotropy of crystals has an important implication in engineering science since it is highly correlated with the possibility to induce microcracks in the materials. The Zener's anisotropic index $A^Z = 2C_{44}/(C_{11} - C_{12})$ can be applied for cubic crystal class only. For a completely isotropic material, A^Z is equal to 1, while any value smaller or larger than 1 indicates anisotropy. The calculated anisotropy factor are $A_{LDA}^Z = 0.475561$, $A_{GGA}^Z = 0.412646$ for $\text{Sr}_2\text{CaMoO}_6$, and $A_{LDA}^Z = 0.4873$, $A_{GGA}^Z = 0.581972$ for Sr_2CaWO_6 , respectively. The mechanical properties of Sr_2CaWO_6 are highly anisotropic.

The Debye temperature is a fundamental and very important parameter for determining physical properties, such as thermal conductivity versus temperature described by Cahill-Pohl model, and the heat capacity versus temperature described by Debye model. We have calculated the Θ_D from the Bulk modulus and shear modulus data and by using the average sound velocity V_m :

$$\Theta_D = \frac{h}{k_B} \left[\frac{3n}{4\pi} \left(\frac{N_A \rho}{M} \right) \right]^{1/3} v_m \quad (10)$$

where h is Planck's constant, k_B is the Boltzmann's constant, N_A the is Avogadro's number, n is the number of atoms per formula unit, M is the molecular mass per formula unit, ρ is the density, and V_m is obtained from:

$$V_m = \left[\frac{1}{3} \left(\frac{2}{V_t^3} + \frac{1}{V_l^3} \right) \right]^{-1/3} \quad (11)$$

where V_t is transverse velocity, V_l is longitudinal velocity. For the cubic structure, which are assumed isotropic material, V_t and V_l are calculated from the Navier's equation:

$$V_l = \sqrt{(B + 4G/3)/\rho} \quad V_t = \sqrt{G/\rho} \quad (12)$$

The average transverse and longitudinal sound velocities are shown in Table 1. Once these parameters are known, we can estimate the mean Debye temperature.

3.2 The planar acoustic wave

The Plane acoustic wave velocity is used to describe wave propagation and can be easily measured by experiments,

which is closely linked with the elastic constants. The acoustic wave velocity are usually obtained using the Christoffel equation [21]:

$$k^2 \begin{bmatrix} \alpha & \delta & \varepsilon \\ \delta & \beta & \zeta \\ \varepsilon & \zeta & \gamma \end{bmatrix} \begin{bmatrix} v_1 \\ v_2 \\ v_3 \end{bmatrix} = \rho \omega^2 \begin{bmatrix} v_1 \\ v_2 \\ v_3 \end{bmatrix} \quad (13)$$

where ρ is the density and $v = \frac{\omega}{k}$ is the plane acoustic wave velocity. For the cubic phase, the tensor components are expressed as follows:

$$\begin{cases} \alpha = C_{11}l_1^2 + C_{66}l_2^2 + C_{44}l_3^2, \\ \beta = C_{66}l_1^2 + C_{11}l_2^2 + C_{44}l_3^2, \\ \gamma = C_{44}(l_1^2 + l_2^2) + C_{33}l_3^2, \\ \delta = (C_{12} + C_{66})l_1l_2, \\ \varepsilon = (C_{13} + C_{44})l_1l_3, \\ \zeta = (C_{13} + C_{44})l_2l_3 \end{cases} \quad (14)$$

As Eq. (13) is an equation of the third power with respect to, in the general ρv^2 case for the given direction in a crystal, we have three velocities ρv_i^2 , where ($i=1,2,3$), which are determined by the positive roots of equation (14). There are three eigenvalues (the results have not been displayed in this paper due to the complex of the accurate formulas), namely two transverse waves and a longitudinal wave (quasi-longitudinal, quasi-shear vertical and quasi-shear horizontal). Figure 2 shows the changes in the acoustic wave velocity of each materials in different crystal orientations. One can see the value of transverse waves velocities is obviously larger than that of a longitudinal wave velocity. The anisotropy of the three dimensional transverse waves velocities is stronger than the longitudinal wave velocity. The three dimensional case of $\text{Sr}_2\text{CaMoO}_6$ is stronger than Sr_2CaWO_6 , indicating that $\text{Sr}_2\text{CaMoO}_6$ has the more significant degree of anisotropy of lattice vibration.

In order to estimate the value of plane acoustic velocities along different crystal orientations, the plane acoustic velocities of the transverse and longitudinal acoustic waves for $\text{Sr}_2\text{CaMoO}_6$, and Sr_2CaWO_6 were calculated in [100], [110], and [111] crystal orientations, respectively. The calculation formulas are as follows [22–26]:

$$\begin{aligned} v_l[100] &= \sqrt{C_{11}/\rho}; \\ v_{t1}[010] &= v_{t1}[010] = \sqrt{C_{44}/\rho}, \end{aligned} \quad (15)$$

$$\begin{aligned} v_l[110] &= \sqrt{(C_{11} + C_{12} + C_{44})2\rho} \\ v_l[1\bar{1}0] &= \sqrt{(C_{11} - C_{12})/2\rho}, \\ v_{t2}[001] &= \sqrt{C_{44}/\rho} \end{aligned} \quad (16)$$

$$v_l[111] = \sqrt{(C_{11} + 2C_{12} + 4C_{44})/3\rho}; \quad (17)$$

$$v_{t1}[11\bar{2}] = v_{t2}[11\bar{2}] = \sqrt{(C_{11} - 2 - C_{12} + C_{44})/3\rho}$$

where C_{ij} is the elastic constant, and ρ is the density.

Table 2: The plane acoustic wave velocities of $\text{Sr}_2\text{CaMoO}_6$ and Sr_2CaWO_6 m/s)

Material		$\text{Sr}_2\text{CaMoO}_6$		Sr_2CaWO_6	
Method		LDA	GGA	LDA	GGA
[100]	[100]	7631.50	6589.46	7060.87	7086.3
	[010],	3278.46	3118.88	3074.74	2812.83
	[001]				
[110]	[110]	6807.13	6036.04	6296.37	6241.30
	[1 $\bar{1}$ 0]	4759.31	4088.35	4434.60	4378.79
	[001]	3278.46	3118.88	3074.74	2818.83
[111]	[111]	6509.18	5839.93	6020.00	5932.95
	[11 $\bar{2}$]	4322.43	3792.83	4032.59	3926.82

4 Conclusions

In this work, we calculated the elastic properties and plane acoustic velocity of the double perovskites $\text{Sr}_2\text{CaMoO}_6$ and Sr_2CaWO_6 by using a pseudopotential plane-wave (PPPW) method with GGA. Some significant conclusions can be drawn as follows: the calculated Lattices are in agreement with experimental data. Elastic constants derived the Young's modulus E , shear modulus G , bulk modulus B , and Poisson's ratio are around 0.25. The results show the value of universal Young's modulus is larger than that of the bulk modulus. Poisson's ratio indicates strong incompressibility for Sr_2CaWO_6 , and $\text{Sr}_2\text{CaMoO}_6$ material. The magnitude of two transverse waves velocities is obviously larger than that of a longitudinal wave velocity, the anisotropy of the three dimensional transverse waves velocities of $\text{Sr}_2\text{CaMoO}_6$ and Sr_2CaWO_6 is stronger than that of the longitudinal wave velocity from the three dimensional. The value of plane acoustic velocities of $\text{Sr}_2\text{CaMoO}_6$ and Sr_2CaWO_6 in [100], [110], and [111] directions were calculated.

To the best our knowledge, among the crystal structures which we synthesized and researched, very few reported the elastic properties and plane acoustic velocity. Therefore the calculated elastic and plane acoustic velocities of Sr_2CaWO_6 , and $\text{Sr}_2\text{CaMoO}_6$ have not been compared with the experimental results. So, it is assumed to be the first theoretical prediction of these properties, as all

the research awaits for experimental confirmation. Hopefully, this work and conclusions can be considered as a foresight study and stimulating matter for further work on Sr_2CaWO_6 and $\text{Sr}_2\text{CaMoO}_6$.

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References

- [1] Sharma G., Narula A.K., Eu^{3+} , Yb^{3+} , and $\text{Eu}^{3+}\text{-Yb}^{3+}$, Complexes with Salicylic Acid and 1,10-Phenanthroline, Synthesis, Photoluminescent Properties and Energy Transfer, *J. Fluorescence*, 2015, 25(2), 355-360.
- [2] Li Y., Liu T., Ye S. et al., Tailored upconversion emission of Eu in SrCa(W,Mo)O_4 , Yb, Eu by a laser an electronic polarization mechanism, *J. Mat. Chem. C*, 2015, 3(19), 4997-5003.
- [3] Sharma K.G., Singh N.R., Synthesis and luminescence properties of CaMoO_4 , Dy^{3+} ($M = \text{W, Mo}$) nanoparticles prepared via an ethylene glycol route, *New J. Chem.*, 2013, 37(9), 2784-2791.
- [4] Guo J., Zhou D., Wang L. et al., Infrared spectra, Raman spectra, microwave dielectric properties and simulation for effective permittivity of temperature stable ceramics $\text{AMoO}_4\text{-TiO}_2$ ($A = \text{Ca, Sr}$), *Dalton Transactions*, 2013, 42(5), 1483-91.
- [5] Ilhan S., Kalpakli A.O., Kahraman C. et al., The investigation of dissolution behavior of gangue materials during the dissolution of scheelite concentrate in oxalic acid solution, *Hydrometallurgy*, 2013, 136(4), 15-26.
- [6] Goel A., McCloy J.S., Jr C.F.W. et al., Structure of Rhenium-Containing Sodium Borosilicate Glass, *International Journal of Applied Glass Science*, 2013, 4(1), 42-52.
- [7] Kang F., Peng M., Yang X. et al., Broadly tuning Bi^{3+} emission via crystal field modulation in solid solution compounds $(\text{Y,Lu,Sc})\text{VO}_4$, Bi for ultraviolet converted white LEDs, *J. Mat. Chem. C*, 2014, 2(30), 6068-6076.
- [8] Ansari A.A., Parchur A.K., Alam M. et al., Influence of Surface Coating on Structural and Photoluminescent Properties of CaMoO_4 , Pr Nanoparticles, *J. Fluorescence*, 2014, 24(4), 1253-1262.
- [9] Chen Y., Park S.W., Moon B.K. et al., Effect of sodium citrate on the shape and photoluminescence properties of CaWO_4 , Eu^{3+} superstructures synthesized by the hydrothermal method, *Crys-tengcomm*, 2013, 15(41), 8255-8261.
- [10] Chouard N., Caurant D., Majérus O. et al., Effect of MoO_3 , Nd_2O_3 , and RuO_2 , on the crystallization of soda-lime aluminoborosilicate glasses, *J. Mat. Sci.*, 2015, 50(1), 219-241.
- [11] Saraf R., Shivakumara C., Dhananjaya N. et al., Photoluminescence properties of Eu^{3+} activated CaMoO_4 , phosphors for WLEDs applications and its Judd-Ofelt analysis, *J. Mat. Sci.*, 2015, 50(1), 287-298.
- [12] Wang M., Chen Z., Chen D. et al., Structural, elastic and thermodynamic properties of A15-type compounds V_3X ($X = \text{Ir, Pt and Au}$) from first-principles calculations, *Modern Phys. Lett. B*, 2016, 30(35), 1650414.
- [13] Guo Z.C., Luo F., Cheng Y., Phase transition and thermodynamic properties of beryllium from first-principles calculations, *Comp. Mat. Sci.*, 2014, 84(1), 139-144.
- [14] Liu S., Zhan Y., Insight into structural, mechanical and thermodynamic properties of zirconium boride from first-principles calculations, *Comp. Mat. Sci.*, 2015, 103, 111-115.
- [15] Niu Z.W., Cheng Y., Zhang H.Y. et al., First-Principles Investigations on Structural, Phonon, and Thermodynamic Properties of Cubic CeO_2 , *Int. J. Thermophys.*, 2014, 35(8), 1601-1612.
- [16] Tao X., Zhu J., Guo H. et al., Phase stability, thermodynamic and mechanical properties of AlZr_2 , FeZr_2 , and Al_2FeZr_6 from first-principles calculations, *J. Nucl. Mat.*, 2013, 440(1-3), 6-10.
- [17] Pu C.Y., Wang L., Lin-Xia L. et al., Pressure-induced structural transition and thermodynamic properties of NbSi_2 from first-principles calculations, *Acta Physica Sinica*, 2015, 64(8), 1-2.
- [18] Yang T., Liu D., Ji J. et al., First-principles calculations for transition phase, mechanical and thermodynamic properties of ZnS under extreme condition, *Int. J. Modern Phys. B*, 2017, 31(5), 1750028.
- [19] Pu C., Zhou D., Song Y. et al., Phase transition and thermodynamic properties of YAg alloy from first-principles calculations, *Comp. Mat. Sci.*, 2015, 102(8), 21-26.
- [20] Zhang X., Zhao X., Zheng B. et al., First-Principles Study of Thermodynamical and Elastic Properties of η' -(Cu,Co) $_6\text{Sn}_5$ Ternary Alloys, *J. Electr. Mat.*, 2016, 45(10), 4919-4927.
- [21] Yan H.Y., Zhang M.G., Huang D.H. et al., First-principles study of elastic and thermodynamic properties of orthorhombic OsB_4 under high pressure, *Solid State Sci.*, 2013, 18(22), 17-23.
- [22] Yuan J., Yu N., Xue K. et al., Stability, electronic and thermodynamic properties of aluminene from first-principles calculations, *Appl. Surf. Sci.*, 2017, 409, 85-90.
- [23] Zhang B., Investigations of the magnetic, mechanical and thermodynamic properties of cubic phase LaMO_3 ($M = \text{Ti-Fe}$), *Phil. Mag. Lett.*, 2017, 97(5), 169-179.
- [24] Xu C., Li Q., Liu C.M. et al., Structural stabilities, elastic and electronic properties of chromium tetraboride from first-principles calculations, *Int. J. Modern Phys. B*, 2016, 30(17), 1650098.
- [25] Planas M.I.G., Klymchuk T., Perturbation analysis of a matrix differential equation $x = \text{ABx}$, *Appl. Math. Nonlinear Sci.*, 2018, 3, 97-104.
- [26] Baig A.Q., Naeem M., Gao W., Revan and hyper-Revan indices of Octahedral and icosahedral networks, *Appl. Math. Nonlinear Sci.*, 2018, 3(1), 33-40.