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First principles investigations of HgX (X=S, Se and Te)

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ABSTRACT

Purpose: The aim of this study is to determine the structural, and mechanical properties of Hg chalcogenide materials (HgX; X=S, Se, Te) in the zinc-blende structure which are presented as promising candidates for modern optoelectronic and spintronic applications. The dependence of elastic constants of pressure for three materials are evaluated. Moreover, isotropic mechanical properties such as bulk modulus, shear modulus, Young's modulus and Poisson's ratio are obtained.

Design/methodology/approach: First principles calculations based on Density Functional Theory are performed by employing Projector Augmented Waves potentials. The electronic exchange and correlation function is treated by using Generalized Gradient Approximation parametrized by Perdew, Burke and Ernzerhof (PBE96).

Findings: Calculated results of structural and mechanical properties are in good agreement with those of experimental and other theoretical studies. This three materials in zinc-blende structure are mechanically stable. İsotropic mechanical properties are also obtained. Resistance against both linear strain and shear strain and ductility decrease as we go into the sequence of HgS–>HgSe–>HgTe. The wave velocities and Debye temperatures calculated for this materials. Debye temperatures are founded for HgS, HgSe and HgTe as 306.21 K, 264.30 K and 240.19 K, respectively

Research limitations/implications: Calculation speeds of the computers and data storage are some limitations. Also, the lack of experimental data hinder for the comparison of our results.

Practical implications: Obtaining high pressure elastic constants by calculations is preferable since it is very difficult or even impossible to measure them by experimentally.

Originality/value: There are only restricted number of investigation of elastic constants of mercury chalcogenides both theoretically and experimentally.

Keywords: Ab initio calculations; Density functional theory; Elastic constants; Structural properties

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MATERIALS

1. Introduction

The mercury chalcogenides, HgX (X=S, Se, Te), which belong to the IIA-VIB group compounds attract attention in recent researches. It is possible to encounter state of the art applications of HgX compounds as new methods to reduce the toxicity of mercury are being improved. They exhibit semiconductor or semimetalic character since they have inverted band gap [1]. HgS in the structure of zinc-blende (ZB) is used to produce nanocrystals or thin films [2]. Topological insulators, optoelectronic and spintronic applications, photovoltaic/photoconductive devices IR detectors and emitters, ohmic contact and removing mercury from exhaust gases, are some examples of their technological applications of mercury chalcogenides [3-7].

It has been observed that HgSe and HgTe are stable in ZB [8,9], while HgS crystallizes in the cinnabar phase [8] and/or ZB structure [10] under ambient condition. Furthermore, some experimental studies show that HgS are stable in ZB structure under the applying pressure [11], keeping the temperature above 344°C [2] or adding small amounts of Fe (~1%) [16]. In this study, we have performed ab-initio simulations to clarify the structural properties of HgS, HgSe and HgTe at ambient conditions. Our results support that HgSe and HgTe are stable in ZB structure, while HgS are found in cinnabar structure. Moreover, we obtain the pressure induced phase transition from cinnabar to ZB structure at 0.86 GPa. As seen, this phase transition takes place at very small pressure. Therefore, we accept the ZB structure as a stable phase for HgS material at ambient conditions in our calculations.

Some experimental studies concerning with structural properties, high pressure phase transitions and elastic constants of HgX chalcogenides have been performed [8-15]. On the other hand, restricted number of theoretical works have been carried out as well [16-23]. While Boutaiba el al. [18] have explored structural and transport properties of ZnX, CdX and HgX (X=S, Se, Te) compounds, Tan et al. [20] have reported phase transitional and vibrational properties of ZB XTe (X=Zn, Cd, Hg) materials in their theoretical work. Ullah et al. [19] have investigated some structural, electronic and optical properties of mercury chalcogenides under pressure. While the structural properties of HgSe and HgTe have been theoretically analyzed by Lu et al. [21] and Hassan et al. [17], their mechanical properties have been predicted by Shafaay et al. [22]. Moreover, the only study including the pressure dependence of elastic constants of mercury chalcogenides are given by Varshney et al. [23].

As we see, there are only restricted number of investigation of elastic constants of mercury chalcogenides both theoretically and experimentally. In this study, therefore, our main aim is to understand the physical behaviour of these materials in the ZB phase under the atomic level by performing ab-initio calculations based on DFT. To achieve our goal, we have obtained lattice constant, bulk modulus and its first pressure derivative as structural properties, and second order elastic constants and their pressure dependence as mechanical properties. In addition, isotropic mechanical properties, such as bulk modulus, shear modulus, Young's modulus and Poisson's ratio, and Debye temperature for HgS, HgSe and HgTe materials are predicted.

2. Material and method

First principles total energy calculations have been performed within DFT by using the Vienna ab initio simulation package (VASP) [24-26] containing Projector Augmented Wave pseudo potential (PAW) method [27]. The electronic exchange-correlation energy is described within Generalized Gradient Approximation (GGA) parameterized by Perdew-Burke-Ernzerhof (PBE) [28]. Kinetic energy cut-off is converged at 450 eV, 400 eV and 500 eV for HgS, HgSe and HgTe respectively, by taking energy difference threshold as 10^{-5} eV per formula unit. Meshes of k-points for Brillouin zone integrations are obtained as 8x8x8 for HgS and as 12x12x12 for HgSe and HgTe materials using Monkhorst-Pack method [29]. In the cubic ZB (B3) structure (cFB, Space Group F$\bar{4}$3m, S.G. No 216, Z=1), Hg atom occupies Wyckoff 4a sites at (0, 0, 0) and X (X=S, Se, Te) atoms are at the Wyckoff 4c (1/4, 1/4, 1/4) in the primitive unit cell [30].

Total energy data calculated are fitted to the 3rd order Birch-Murnaghan equation of states (EOS) in order to obtain structural optimizations [31].

$$E(V) = E_0 + \frac{9V_0B_0}{16}\left\{\left[\left(\frac{V_0}{V}\right)^{\frac{2}{3}}-1\right]^3 B_0' + \left[\left(\frac{V_0}{V}\right)^{\frac{2}{3}}-1\right]^2\left[6-4\left(\frac{V_0}{V}\right)^{\frac{2}{3}}\right]\right\} \quad (1)$$

where E_0 is the total energy, V_0 is the equilibrium volume, B_0 is the bulk modulus at 0 GPa pressure, and B_0' is the first pressure derivative of bulk modulus.

3. Results and discussion

3.1 Structural properties

Structural optimizations have been carried out by taking experimental lattice parameters as starting point. Structural

parameters calculated, such as lattice constant a, bulk modulus B_0 and its first pressure derivative B_0' of HgX (X=S, Se, Te) in the ZB phase are given in Table 1, in comparison with available experimental and other theoretical results.

Table 1.
Lattice constant a (A^0), bulk modulus B_0 (GPa) and its first pressure derivative B_0' of HgX (X=S, Se, Te) in the structure of ZB at 0 K and 0 GPa

Material	Structural properties	Present	Experiment	Others
HgS	a	5.988	5.851[a]	6.197[b], 5.88[c], 5.863[d]
	B_0	50.189		47.53[b], 65.4[c], 63.6[d]
	B_0'	4.61		
HgSe	a	6.276	6.084[e]	6.464[b], 6.11[c], 6.115[d]
	B_0	42.890	57.6[f]	40.21[b], 53.9[c], 53.93[d]
	B_0'	5.21		4.88[g]
HgTe	a	6.662	6.461[e], 6.453[h]	6.893[b], 6.51[c], 6.521[d]
	B_0	47.210	47.6[i], 42.3[j]	33.36[b], 43.8[c], 43.2[d]
	B_0'	6.31	2.1[j]	5.79[g]

Our calculated lattice constants are in good agreement with experimental and available other theoretical results. The present and other theoretical results obey the limitations of DFT, because they are evaluated as 1-3% greater than experimental ones.

3.2 Mechanical properties

Elastic stiffness constants and compliances

C_{ij} second order elastic stiffness constants are obtained through the total energy calculations of the strained system.

Taylor expansion of the energy of the strained system is as follows:

$$E(V,\varepsilon) = E(V_0) + V_0 \sum_i \sigma_i \varepsilon_i + \frac{V_0}{2}\sum_{ij} C_{ij}\, \varepsilon_i \varepsilon_j + \cdots, \qquad (2)$$

where i, j=1, 2, …, 6 (Voight's notation). $E(V,\varepsilon)$ and $E(V_0)$ are total energies of strained and unstrained structures, respectively. V is the deformed volume and V_0 is the equilibrium volume at zero pressure, δ_i is the stress and ε is the strain tensor. C_{ij} are the second-order elastic stiffness constants. The third term in Eq. (2) is used to calculate second-order elastic stiffness constants. A deformation parameter δ changing from -0.03 to 0.03 by the steps of 0.01 is used to obtain strain tensors. Then, total energy versus δ data are fitted to a third-order polynomial function. Hence, the elastic constants are obtained by taking the second order coefficient of this fit.

A cubic crystal has three independent elastic moduli C_{11} C_{12} and C_{44} because of the symmetry. Therefore, we need to three different strain tensors to reach these elastic constants. Two of them, tetragonal shear strain ε_1 and pure shear strain ε_2, are volume conserving, while the third one ε_3 gives the bulk modulus. Applied strains and their corresponding energies after deformation are the following [32]:

$$\varepsilon_1 = \begin{pmatrix} \delta & 0 & 0 \\ 0 & -\delta & 0 \\ 0 & 0 & \delta^2/(1-\delta^2) \end{pmatrix},$$

$$E(\delta) = E_0 + 2C_S V_0 \delta^2 + O(\delta^4), \qquad (3)$$

where $C_S=(C_{11}-C_{12})/2$ is tetragonal shear elastic constants.

$$\varepsilon_2 = \begin{pmatrix} 0 & \delta & 0 \\ \delta & 0 & 0 \\ 0 & 0 & \delta^2/(1-\delta^2) \end{pmatrix},$$

$$E(\delta) = E_0 + 2C_{44} V_0 \delta^2 + O(\delta^4), \qquad (4)$$

where C_{44} is the pure shear elastic constant.

$$\varepsilon_3 = \begin{pmatrix} \delta & 0 & 0 \\ 0 & \delta & 0 \\ 0 & 0 & \delta \end{pmatrix} \text{ and } E(\delta) = E_0 + \frac{9}{2}BV_0\delta^2 + O(\delta^4), \qquad (5)$$

where $B=(C_{11}+2C_{12})/3$ is the bulk modulus.

S_{ij} elastic compliances are also calculated from elastic constants C_{ij} in order to reach isotropic mechanical properties [32]:

$$S_{44} = \frac{1}{C_{44}}, \; S_{11} - S_{12} = \frac{1}{C_{11}-C_{12}},$$

$$S_{11} + S_{12} = \frac{C_{11}}{(C_{11}-C_{12})(2C_{12}+C_{11})}. \qquad (6)$$

Our results for elastic constants and their elastic compliances of three materials are collected in Table 2. These values of the experimental and other theoretical studies are also given in the same table to compare our results with them. While the values of elastic constants of HgSe and HgTe are in good agreement with those of experimental studies [14,36], we have not found any experimental result of HgS to compare. Our results of all structure are compatible with those of the theoretical study reported by Shafaay [22]. Moreover, our calculations of elastic constants show better agreement with the experiment than those of other study [23]. Pressure behaviours of elastic constants and bulk modulus of HgS, HgSe and HgTe are displayed in Figs. 1 a-c, respectively. As seen from the figures, as the pressure rises, the elastic constants and bulk modulus increase linearly. The elastic constants calculated in this study obey the mechanical stability criteria which are the following as [37]:

$$C_{11} - C_{12} > 0, \quad C_{44} > 0 \quad \text{and} \quad C_{11} + 2C_{12} > 0 \qquad (7)$$

Isotropic mechanical properties

Isotropic mechanical properties are calculated by Voight-Reuss-Hill (VRH) averaging scheme as given in Ref. 32 and references therein.

Table 2.
Elastic constants C_{ij} (GPa) and elastic compliances S_{ij} (GPa^{-1}) of HgS, HgSe and HgTe, in comparison with available experimental and theoretical results

Materials		C_{11}	C_{12}	C_{44}	B_0	S_{11}	S_{12}	S_{44}
HgS	Present	63.03	46.86	40.76	52.25	0.0433	-0.0185	0.0245
	Experiment							
	Others	79.3[a]	65.3[a]	49.7[a]	63.6[a]			
		22.0[b]	5.0[b]	10.4[b]	35.0[b]			
HgSe	Present	52.69	37.99	33.69	42.89	0.0479	-0.0201	0.0297
	Experiment	62.16[c]	46.40[c]	22.68[c]	51.66[c]			
		69.00[d]	51.05[d]	23.073[d]				
	Others	74.5[a]	50.7[a]	44.1[a]	53.93[a]			
		28.7[b]	9.9[b]	21.4[b]	67.8[b]			
HgTe	Present	44.29	29.49	29.35	34.42	0.0483	-0.0193	0.0341
	Experimental	59.71[e]	41.54[e]	22.59[e]				
	Others	57.0[a]	43.0[a]	25.4[a]	43.2[a]			
		30.9[b]	11.65[b]	20.2[b]	56.8[b]			

[a] Ref. [22], [b] Ref. [23], [c] Ref. [14], [d] Ref. [15], [e] Ref. [36]

Table 3.
The isotropic bulk modulus B (GPa) and shear modulus G (GPa) for polycrystalline HgX (X=S, Se, Te) from the single crystal elastic constants using Voigt, Reuss and Hill's approximations. The Young's modulus E (GPa) and the Poisson's ratio V are predicted from Hill's approximation, along with the other study

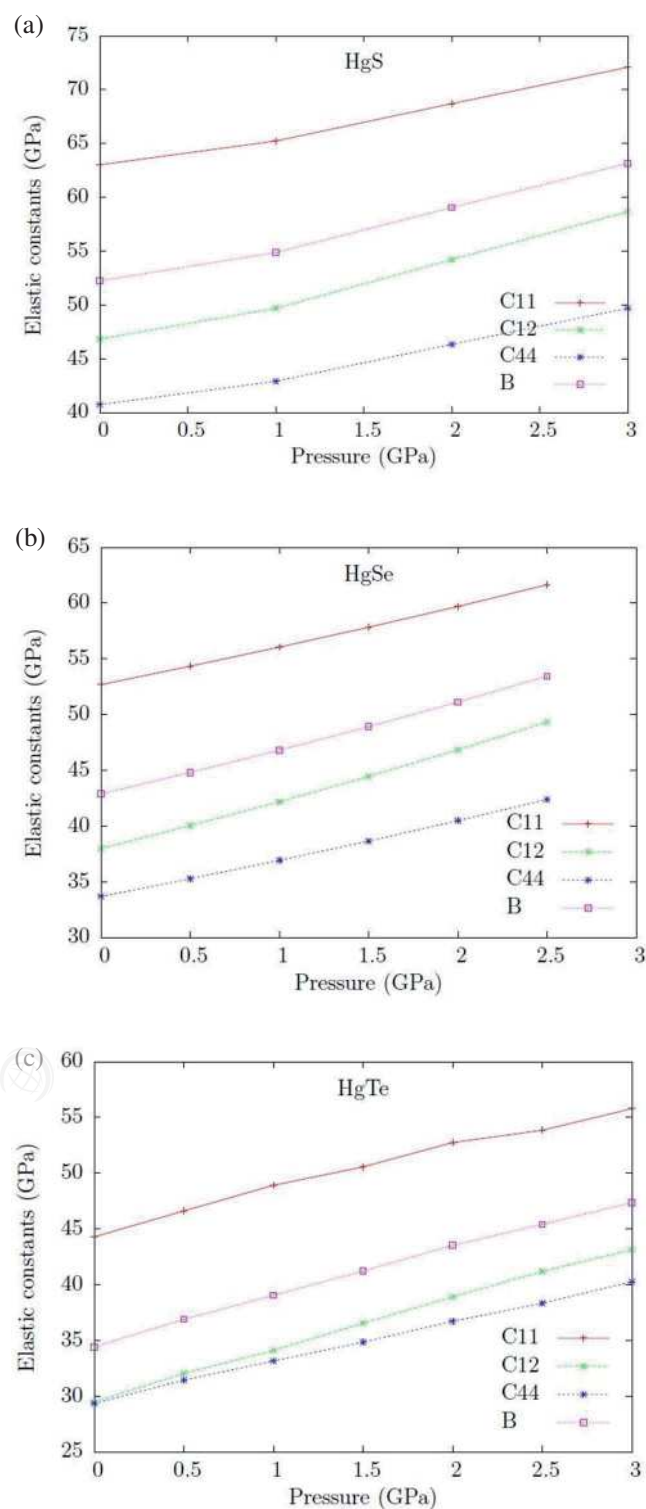| Compound		$B_v=B_R=B$	G_v	G_R	G	B/G	E	v
HgS	Present	52.25	27.69	15.58	21.63	2.42	57.03	0.318
	Other		9.6[a]	9.5[a]	9.6[a]		22.1[a]	1.54[a]
HgSe	Present	42.89	23.15	13.84	18.50	2.32	48.52	0.311
	Other		6.6[a]	2.5[a]	4.6[a]		11.8[a]	1.32[a]
HgTe	Present	34.42	20.57	13.42	17.00	2.02	43.78	0.288
	Other		8[a]	4.4[a]	6.2[a]		15.5[a]	2.49[a]

[a] Ref. [23]

(a)

(b)

(c)

Fig. 1. Elastic constants and bulk modulus as a function of pressure of a) HgS, b) HgSe and c) HgTe in ZB structure

The Voight and Reuss isotropic bulk moduli, which are measure of resistance of a system to change its volume, are the same for cubic systems: $B=B_v=B_R=(C_{11}+2C_{12})/3$. This value is 52.25 GPa, 42.89 GPa and 34.42 GPa for HgS, HgSe and HgTe, respectively. Upper bound of shear modulus is the Voight shear modulus G_V and lower bound is the Reuss shear modulus G_R Shear modulus G is obtained by taking the average of two approximations: $G=(G_R+G_v)/2$. G values are calculated as 21.63 GPa, 18.50 GPa and 17.00 GPa for HgS, HgSe and HgTe, respectively. Calculated isotropic mechanical properties are given in Table 3, along with other theoretical study [23]. The B/G ratio can be interpreted as indication of ductility. If it is greater than the critical value of 1.75, material shows ductile character. This ratio is found above the critical value, which reflects that Hg chalcogenides are ductile.

Listed also in Table 3 are the results for Young's modulus and Poisson's ratio of Hg chalcogenides. Young's modulus E is related to stiffness of an isotropic elastic system against linear strain and Poisson's ratio v is a measure of stability of a material when a shear strain is applied. In our calculations, E values are 57.03 GPa, 48.52 GPa and 43.78 GPa, v values are 0.318, 0.311 and 0.288 for HgS, HgSe and HgTe, respectively. Resistance against both linear strain and shear strain and ductility decrease as we go into the sequence of HgS→HgSe→HgTe.

We are also interested in Debye temperature for three materials considered in this work by using isotropic mechanical properties. For low temperature, we have predicted the Debye temperatures of HgX (X=S, Se, Te) materials from the averaged sound velocity v_M which can be obtained by taking the contribution of longitudinal and transverse elastic wave velocities. The formulas for Young's modulus, Poisson's ratio and Debye temperature are given in Ref [32]. The wave velocities and Debye temperatures predicted for HgX in the ZB structures are collected in Table 4. As seen from the table, Debye temperature for HgS is higher than that for HgSe. Similarly we have found it for HgSe higher than that for HgTe, as confirmed by the other theoretical study [17].

In summary, we have carried out total energy calculations based on DFT to present the comprehensive study including structural, unisotropic and isotropic mechanical properties of mercury chalcogenides in ZB structure. In general, our results presented in this study are compatible with the available experimental and other theoretical studies.

Table 4.
The longitudinal v_l (m/s), transverse v_T (m/s) and average sound velocity v_M (m/s) calculated from isotropic elastic moduli and θ_D (K) Debye temperature evaluated via average sound velocity for mercury chalcogenides, along with other theoretical results [17,23]

	v_l	v_T	v_M	θ_D
HgS	3356	1733	1940	306.21 76.532[b]
HgSe	2998	1569	1755	264.30 231[a] 51.188[b]
HgTe	2782	1518	1693	240.19 211[a] 55.955[b]

[a] Ref. [17], [b] Ref [23]

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