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First-Principles Study of the Structural, Mechanical, Lattice Dynamic, and Thermodynamic Properties of CuBS₂ Semiconductor

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ABSTRACT: Using first principles calculations, we have systematically studied the structural, elastic, mechanical, lattice dynamic, and thermodynamic properties of the CuBS₂ semiconductor. The calculated structural parameters are in good agreement with the experimental values. The obtained elastic constants confirm that the compound is mechanically stable. The B/G ratio of CuBS₂ indicating that this crystal possesses ductile characteristics. Using the ELATE software, 3D and 2D visualizations of anisotropic elastic properties, namely, the maximum and minimum values of Young's modulus (E), shear modulus (G), linear compressibility (β), and Poisson's ratio (ν), have been analyzed. Furthermore, we calculated the elastic anisotropy index (A^U , A_B , and A_G) and the shear anisotropy factor (A_1 , A_2 , and A_3) along different crystal planes. Crucially, the lattice vibration properties of CuBS₂ were investigated, including phonon spectra and phonon state densities. The calculated phonon spectra have no imaginary frequencies throughout the entire Brillouin zone, indicating that the tetragonal CuBS₂ is dynamically stable, and the contributions of different atomic pairs to the vibration modes were analyzed. Based on the calculated phonon dispersion relations, the constant-pressure thermodynamic properties of CuBS₂, including the Debye temperature, Helmholtz free energy, enthalpy, specific heat capacity, and entropy, were computed systematically. The calculated mechanical and thermodynamic parameters provide important theoretical advice for the rational design, synthesis, and industrial application of CuBS₂ materials.

KEYWORDS: CuBS₂; first principles calculations; elastic properties; phonon; thermodynamic properties

1 Introduction

CuBS₂ (copper boron sulfide) is an emerging, high-performance ternary semiconductor material belonging to the chalcopyrite family. This material has promising applications in photovoltaics, thermoelectricity, photocatalysis, and nonlinear optics [1–3]. This novel material has attracted the interest of researchers, and some investigations have been carried out. Experimentally, Kajiki et al. reported the high pressure synthesis of CuBS₂ [4]. Theoretically, researchers computationally revealed the direct band gap nature of CuBS₂ [5–8]. Bagci et al. systematically investigated the structural, electronic, optical, vibrational, and transport properties of the chalcopyrite structured semiconductor CuBS₂, exploring its potential applications in optoelectronics and thermoelectrics [9]. Djoummekh et al. studied the stability and linear/nonlinear optical properties of CuBS₂ via density functional theory (DFT), revealing its potential as a nonlinear optical material [10].

It should be noted that existing theoretical research has primarily focused on the electronic structure and optical properties of this material, and there are few reported studies on its mechanical and vibrational

properties, and thermodynamic properties have not been studied. These material properties directly determine the mechanical stability, machinability, and reliability under thermal conditions. They serve as a bridge between microscopic atomic arrangements and macroscopic engineering applications. For example, a low Poisson's ratio helps materials resist bending fracture on flexible substrates, while excessive anisotropy can lead to cracking during crystal cutting. The Debye temperature can be used to determine the lattice thermal conductivity, which is crucial for the design of thermoelectric materials. This research will use the first-principles method to systematically investigate its structural, elastic, mechanical, lattice dynamic, and thermodynamic properties. The computational results can serve as useful references for the experimental preparation of CuBS₂ materials.

2 Computational Methods

The density function theory is widely used to investigate the physical properties of pure- and doped-crystal materials, yielding numerous novel and reliable results [11,12]. In this work, we used the CASTP code [13,14] which based on the density functional theory to calculate the structural, elastic, lattice dynamic, and thermodynamic properties of CuBS₂ crystal. To ensure the computational efficiency and the reliability of the calculated results, we carried out a convergence test for the plane-wave cutoff energy and the k-point grid within the Brillouin zone, as shown in Fig. 1. First, we fixed the k-point grid at $3 \times 3 \times 2$ and sampled the plane-wave cutoff energy from 250 to 650 eV in increments of 50 eV. It was observed that the system energy converged at 400 eV. Second, in the convergence test of the k-point grid, we set the plane-wave truncation energy to 400 eV and varied the k-point grid size from $4 \times 4 \times 3$ to $11 \times 11 \times 6$. The curves flattened out starting from the $7 \times 7 \times 4$ k-point grid, indicating the convergence of energy. After the convergence testing, in the geometry optimization process, a $7 \times 7 \times 4$ Monkhorst-Pack k-point grid spacing in the Brillouin zone was adopted, and the plane wave cutoff energy was set to 600 eV, the Broyden-Fletcher-Goldfarb-Shanno (BFGS) method was employed [15]. The generalized gradient approximation (GGA) of Perdew-Burke-Ernzerhof (PBE) [16] is adopted to describe the effects of exchange-correlation interactions. Vanderbilt-type ultrasoft pseudopotentials (USP) [17] are used to model electron-ion interactions. Geometric optimization was considered converged when the following criteria were simultaneously satisfied: The total energy discrepancy between consecutive self-consistent field (SCF) cycles was maintained below 1×10^{-6} eV, the maximum Hellmann-Feynman force acting on any ion was constrained to be below 0.01 eV/Å, the maximum ionic displacement was restricted to less than 5×10^{-4} Å, and the maximum stress exerted on any ion was limited to less than 0.02 GPa. Based on the optimized geometric structure, the elastic constants of the crystal were calculated as the second derivatives of the internal energy with respect to the strain tensor.

Phonon calculations were performed using density functional theory (DFT). We employed the finite displacement method [18] and used one large supercell defined by a cutoff radius of 3.5 Å to determine the phonon dispersion relations and phonon density of states (DOS) of the CuBS₂ crystal. From the phonon DOS and within the harmonic approximation, the thermodynamic properties of the material can be derived.

3 Results and Discussions

3.1 Structural Optimization

The CuBS₂ compound belongs to the space group I-42d and possesses a non-centrosymmetric tetragonal structure. The experimental lattice constants of this compound, as referenced in [4], are $a = 5.044$ Å and $c = 8.947$ Å, respectively. In this configuration, a represents the lattice constant along the x/y axes, and c represents the lattice constant along the z axis. As demonstrated in Fig. 2, the conventional unit cell of

CuBS₂ comprises two molecular formulas. The Wyckoff positions of Cu, B, and S are denoted by 4a (0, 0, 0), 4b (0, 0, 0.5) and 8d (0.308, 0.25, 0.125), respectively.

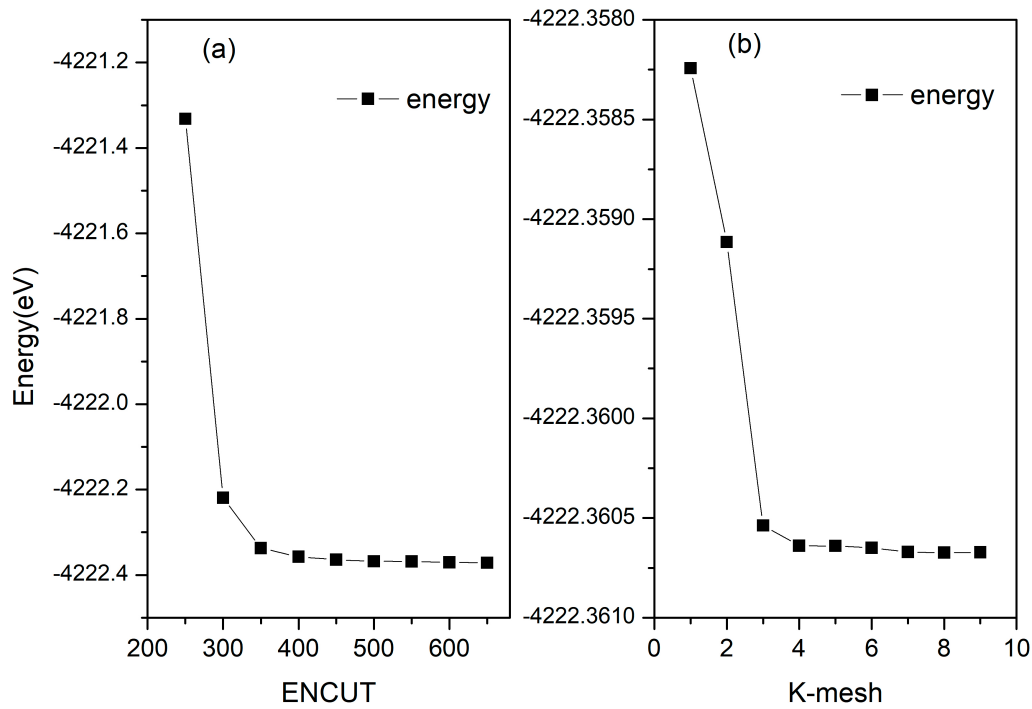


Figure 1: (a) Total energy at different cutoff energy with $3 \times 3 \times 2$, (b) Total energy at different k-mesh with 400 eV.

Using the experimental lattice parameters of CuBS₂ [4] as initial values, geometric optimization was carried out, and the process was completed when the convergence condition was met. The calculated lattice constants a and c are 5.013 and 9.067 Å, respectively, and have deviations of 0.6% and 1.3% compared to the experimental values, which is a favorable agreement by DFT standards. The calculated lattice parameters, along with other experimental and theoretical values from the literature for comparative analysis, are listed in Table 1. Using the optimized crystal structure of CuBS₂, we can further explore the elastic, lattice dynamic, and thermodynamic properties of the material.

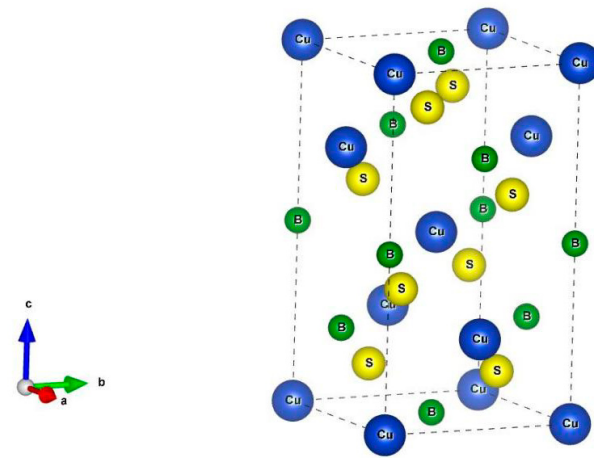


Figure 2: Crystal structure of CuBS₂.

Table 1: The lattice constant a , b (Å), c (Å), η , and the internal parameters u for CuBS₂.

	a, b (Å)	c (Å)	$\eta = c/2a$	u
This work	5.013	9.067	0.904	0.305
Theo. [10]	5.01	9.06	0.904	0.305
Theo. [9]	5.00	9.08	0.908	0.197
Exp. [4]	5.044	8.947	0.887	0.308

3.2 Elastic Properties

The elastic tensor of a solid material is important in two respects. Firstly, it characterises the material's response to applied stress. Secondly, it provides a criterion for assessing structural stability. In consideration of the structural symmetry of the material, the elastic stiffness tensor of the chalcopyrite-structured compound CuBS₂ is comprised of six independent components, denoted by C_{11} , C_{33} , C_{44} , C_{66} , C_{12} , and C_{13} , according to Young's notation. It is evident that, as of the present moment, there is an absence of experimental data concerning the elastic constants of the CuBS₂ crystal. The six independent elastic constants of CuBS₂ have been obtained via first-principles calculations and are listed in Table 2. It is evident that the elastic constants of CuBS₂ exhibit substantial anisotropy, which is attributed to the disparity in bond strength between the Cu-S and B-S chemical bonds. For the chalcopyrite structure, the Born stability criteria for the CuBS₂ crystal are given by C_{11} , C_{33} , C_{44} , $C_{66} > 0$, $C_{11} > |C_{12}|$, $C_{11}C_{33} > C_{13}^2$ and $(C_{11} + C_{12})C_{33} > 2C_{13}^2$. It is evident that the calculated elastic constant values satisfy the mechanical stability requirements for chalcopyrite crystals [19], indicating that CuBS₂ is mechanically stable.

Table 2: The elastic constants C_{ij} (in GPa), bulk modulus B_H , shear modulus G_H , Young's modulus E , the Poisson's ratio ν , and elastic anisotropy factors (A^U , A_B , A_G , A_1 , A_2 and A_3) of CuBS₂ at 0 K.

		C_{11}	C_{12}	C_{13}	C_{33}	C_{44}	C_{66}
CuBS ₂	This work	178.11	84.89	88.06	126.79	83.34	89.83
	Ref. [10]	175.03	83.47	85.98	141.26	80.78	89.52
		B_H	G_H	E	σ		
	This work	110.1	59.6	151.48	0.27		
	Ref. [10]	111.36	65.94	165.21	0.252		
		A^U	A_B	A_G	A_1	A_2	A_3
	This work	1.249	0.0142	0.109	2.588	2.588	1.927

The isotropic elastic moduli of the polycrystalline aggregate were calculated from the anisotropic single-crystal elastic stiffness tensor using the Voigt and Reuss approximations [20,21].

$$B_V = \frac{1}{9}(2C_{11} + C_{33} + 2C_{12} + 4C_{13}) \quad (1)$$

$$B_R = \frac{(C_{11} + C_{12})C_{33} - 2C_{13}^2}{C_{11} + C_{12} + 2C_{33} - 4C_{13}} \quad (2)$$

$$G_V = \frac{1}{15}(2C_{11} + C_{33} - C_{12} - 2C_{13} + 6C_{44} + 3C_{66}) \quad (3)$$

$$G_R = 15/(8s_{11} + 4s_{33} - 4s_{12} - 8s_{13} + 6s_{44} + 3s_{66}) \quad (4)$$

where $s = C^{-1}$ is the elastic compliance matrix.

Since the Voigt and Reuss isotropic average values of the bulk modulus and shear modulus represent the upper and lower bounds, respectively. Hill [22] proposed that the bulk modulus and shear modulus of polycrystalline materials should be approximated as the arithmetic mean of these two values, that is:

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

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

The Young's modulus can be expressed as follows: $E = (9B_H G_H)/(3B_H + G_H)$. After substituting the obtained values of B_H and G_H into the formula, we can yield that the Young's modulus is 151.48 GPa. The Poisson's ratio ν is then determined by the formula: $\nu = (3B_H - 2G_H)/(6B_H + 2G_H)$. Similarly, the Poisson's ratio ν of this material can be obtained as 0.27. According to reference [23], it can be concluded that this material is an ionic material. According to Pugh's rule [24], when the B/G ratio exceeds 1.75, the material exhibits ductility; conversely, when the B/G ratio is below 1.75, it becomes brittle. Calculations yield a B/G ratio of 1.87 for CuBS₂, indicating this material possesses excellent ductility. This characteristic has an indirect connection to Young's modulus and elastic modulus anisotropy. A comparison was made between the elastic parameters B_H , G_H , E , and ν of the CuBS₂ crystal and those of the chalcopyrite crystal CuInS₂ (82.4 GPa, 33.8 GPa, 89.2 GPa, and 0.32, respectively) [25]. It can be observed that CuBS₂ demonstrates a higher degree of resistance to deformation.

The anisotropy of the crystalline material can be directly observed by displaying the Young's modulus (E), the linear compressibility (β), the shear modulus (G), and the Poisson ratio (ν) of the two- and three-dimensional graphs. Using the ELATE code [26], a free program, we may create 2D and 3D graphs of different elastic parameters based on the computed elastic constant matrix. Elastic isotropy is indicated by circular and spherical plots, however, the greater the disparity between 2D graphs and circles, or 3D graphs and spheres, the more pronounced the elastic anisotropy becomes. As illustrated in Figs. 3 and 4, the elastic parameters E , β , G , and ν of CuBS₂ crystals with a tetragonal crystal system exhibit anisotropic behaviour when viewed from both three-dimensional and two-dimensional perspectives (xy -, xz -, and yz -planes). The minimum and maximum values of the parameters are denoted by the green and blue curves, respectively. A thorough examination of the two-dimensional and three-dimensional images of the elastic parameters of CuBS₂ crystals was conducted, resulting in the discovery that the degree of anisotropy for each elastic parameter increases in the following order: $\beta < E < G < \nu$.

To quantitatively analyze the elastic anisotropy of CuBS₂ semiconductor, we employed the formula from reference [27] to calculate the elastic anisotropy index (A^U , A_B , A_G) and the shear anisotropy factors (A_1 , A_2 , and A_3) for the $\langle 100 \rangle$, $\langle 010 \rangle$, and $\langle 001 \rangle$ crystal planes of CuBS₂,

$$A^U = 5G_V/G_R + B_V/B_R - 6 \quad (7)$$

$$A_B = (B_V - B_R)/(B_V + B_R) \quad (8)$$

$$A_G = (G_V - G_R)/(G_V + G_R) \quad (9)$$

$$A_1 = A_2 = 4C_{44}/(C_{11} + C_{33} - 2C_{13}) \quad (10)$$

$$A_3 = 4C_{66}/(C_{11} + C_{22} - 2C_{12}) = 2C_{66}/(C_{11} - C_{12}) \quad (11)$$

Because CuBS₂ semiconductor is tetragonal symmetry, hence, $C_{11} = C_{22}$. The results are presented in Table 2. Here, A^U represents the overall anisotropy degree of the material, while A_B and A_G denote the percentage of compressive anisotropy and shear anisotropy, respectively. The calculated elastic anisotropy index A^U , A_B , and A_G , along with the shear anisotropy factors A_1 , A_2 , and A_3 of CuBS₂ are all given in Table 3. As is widely known, If the elastic anisotropy index satisfies $A^U = A_B = A_G = 0$, this means the material is isotropic. The elastic anisotropy indexes shown in Table 3 are all non-zero, indicating that CuBS₂ has a strong degree of anisotropy.

It is found that A_B is much smaller than A_G , indicating that the compressive anisotropy is very small, and the anisotropy of the material mainly originates from the shear modulus. For a material in tetragonal symmetry, the shear anisotropy factors $A_1 = A_2$. From Table 3, A_1 , A_2 and A_3 , all are greater than 1. This indicates that on these crystal planes, the shear resistance is low, making sliding easy, and the material exhibits ductility.

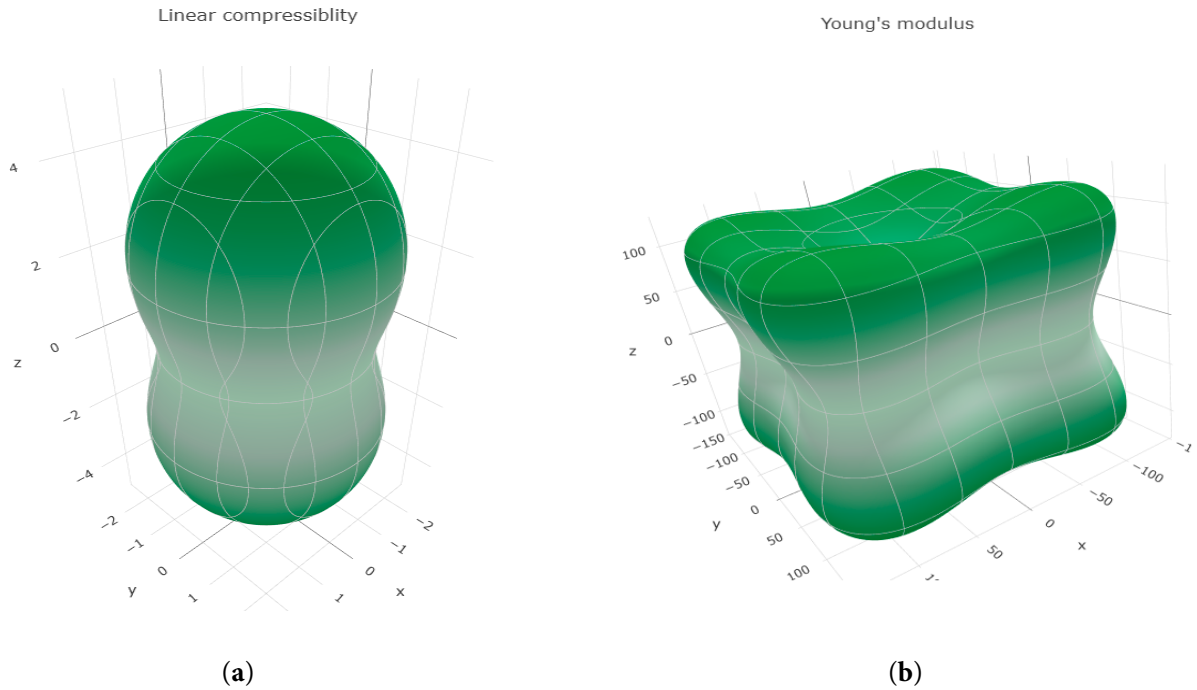


Figure 3: Cont.

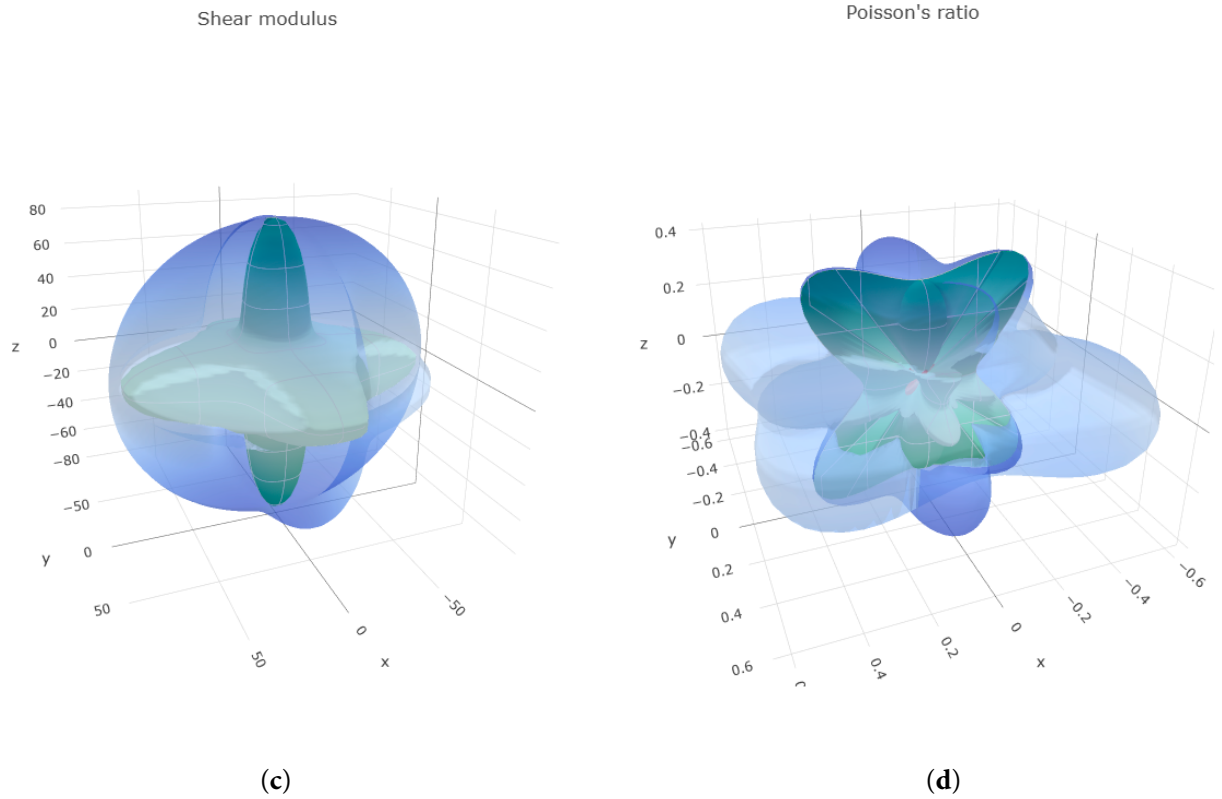


Figure 3: Three-dimensional (3D) surface construction of linear compressibility (a), Young modulus (b), Shear modulus (c), and Poisson's ratio (d) of CuBS_2 .

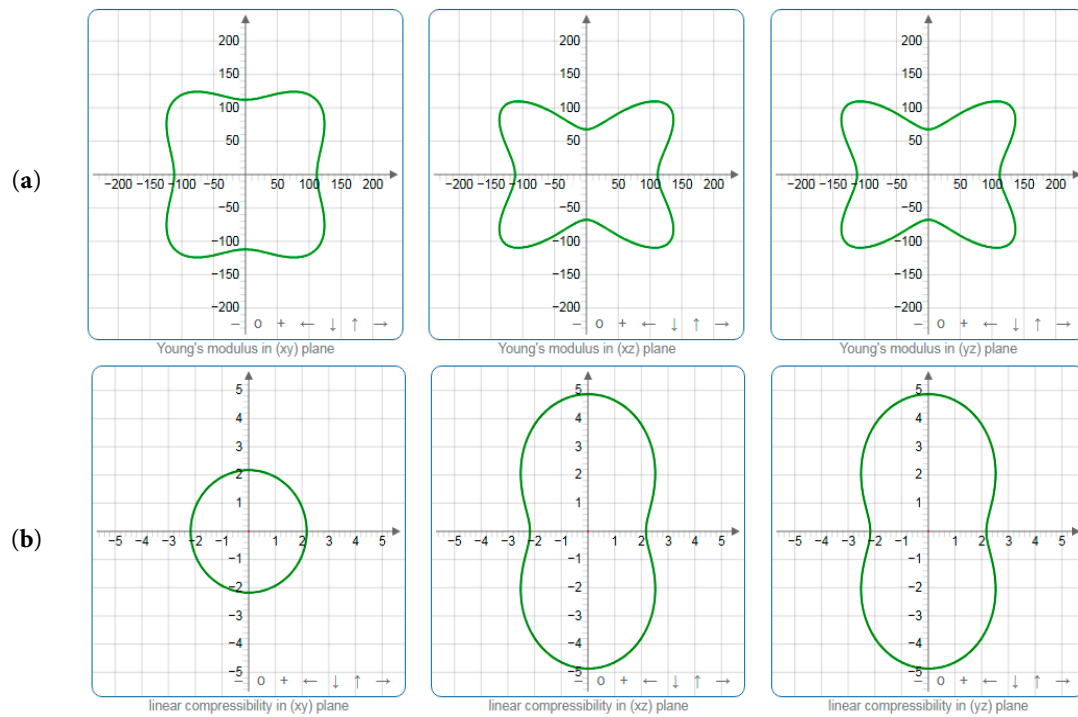


Figure 4: Cont.

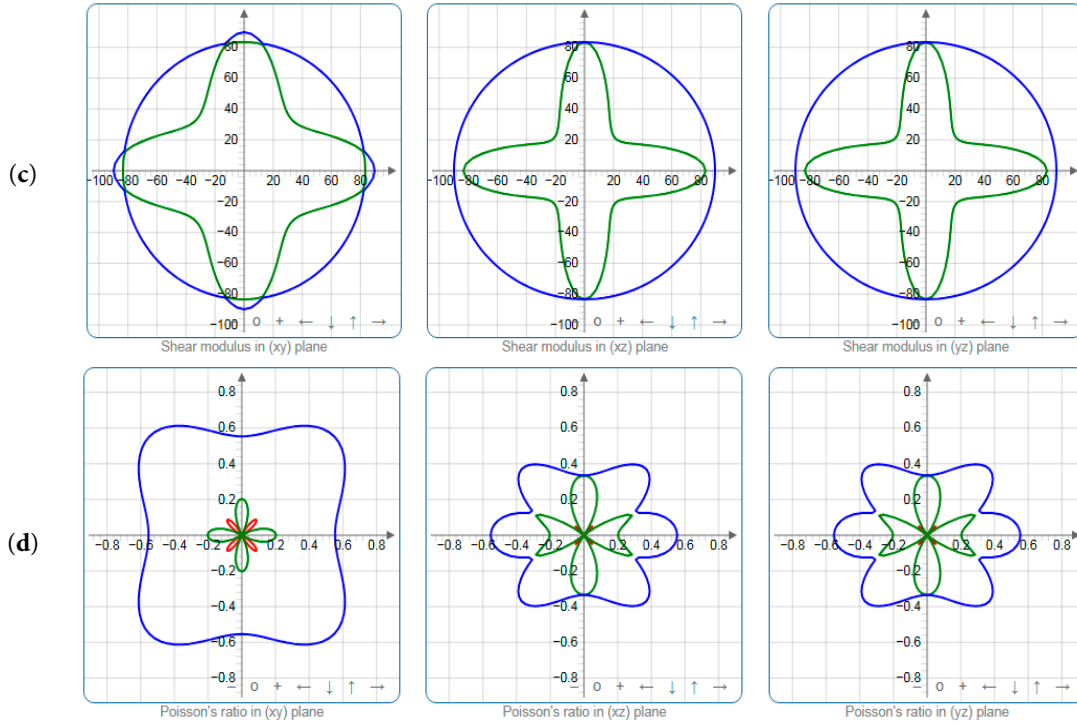


Figure 4: Projections in (xy, xz and yz) plane of linear compressibility (a), Young modulus (b), shear modulus (c), and Poisson's ratio (d) of CuBS₂.

3.3 Lattice Dynamical Properties

The phonon spectrum serves as a bridge that links the microscopic atomic vibrations of a material to its macroscopic properties. By using the finite-displacement method based on DFT, we obtained the phonon spectrum along high-symmetry points in the Brillouin zone of CuBS₂. Figs. 5 and 6 illustrate the phonon band structure and phonon density of states of CuBS₂, respectively. Fig. 5 shows that there are no imaginary frequencies throughout the entire Brillouin zone, indicating that the tetragonal CuBS₂ is dynamically stable. Two phonon band-gaps are present across the entire vibrational spectrum, located in the frequency ranges of 120–160 cm⁻¹ and 416–533 cm⁻¹, respectively. One can see that, the phonon spectrum reveals no distinct bandgap between the acoustic vibration branch (black line) and the low-frequency optical vibration branch (red line), in fact, the two branches even partially overlap, indicating that energy exchange between them is readily achievable. As shown in Fig. 6, the high-frequency vibrational peaks (>533 cm⁻¹) are primarily contributed by B atoms. The low-frequency acoustic and optical branches primarily originate from the vibrations of Cu atoms, while the mid-frequency optical branch is mainly due to the contribution of S atoms, with some contributions from B and Cu atoms.

According to the lattice dynamics theory, if the primitive cell of a material contains n atoms, its vibrational spectrum contains $3n$ vibrational branches. The CuBS₂ semiconductor material has 8 atoms in the primitive cell. The vibrational spectrum of this crystal contains 24 vibrational modes, of which 3 branches are acoustic modes and the remaining 21 branches are optical vibrational modes. At the wave vector $K = 0$, the irreducible representation of these 24 vibrational modes is classified as: $\Gamma = 1A_1 + 2A_2 + 3B_1 + 4B_2 + 7E$. The three acoustic modes are B_2 and E , which have a frequency of 0 at the Γ point. Among the remaining 21 optical modes, there are 9 infrared-excited modes ($3B_2$ and $6E$) and 19 Raman-excited modes (A_1 , $3B_1$, $3B_2$, and $6E$). It can be seen that 9 of these modes, namely $3B_2$ and $6E$, are simultaneously

Raman and infrared excited. The results of our calculations for the optical vibration branches, along with the theoretical values from other researchers, are listed in Table 3. As shown in Table 3, the frequency variation patterns of the optical vibration modes calculated at the Γ point in the Brillouin zone are consistent with those reported in reference [9], and each mode exhibits slightly lower frequencies, this phenomenon may be due to the temperature-dependent volume change was not considered in the calculations.

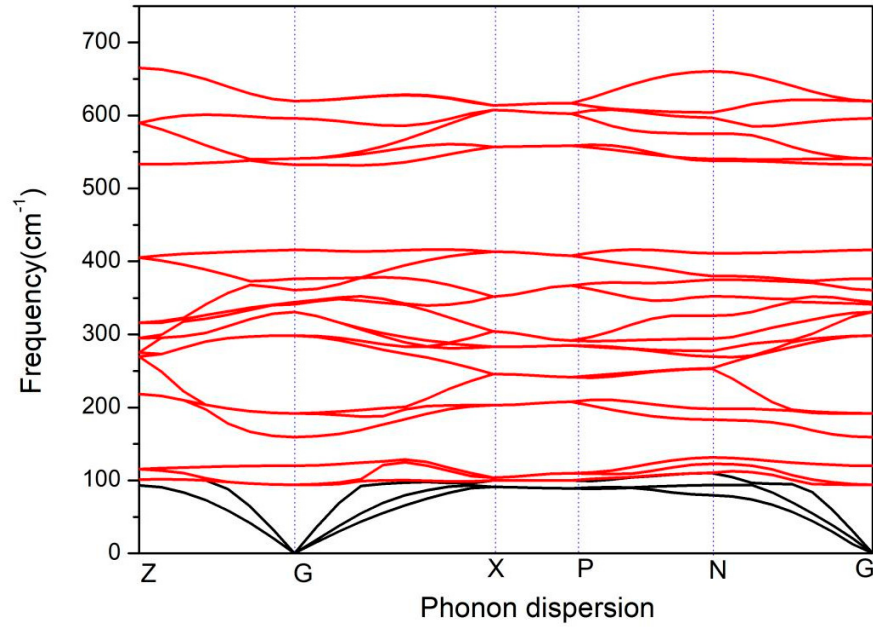


Figure 5: Phonon band structure of CuBS₂.

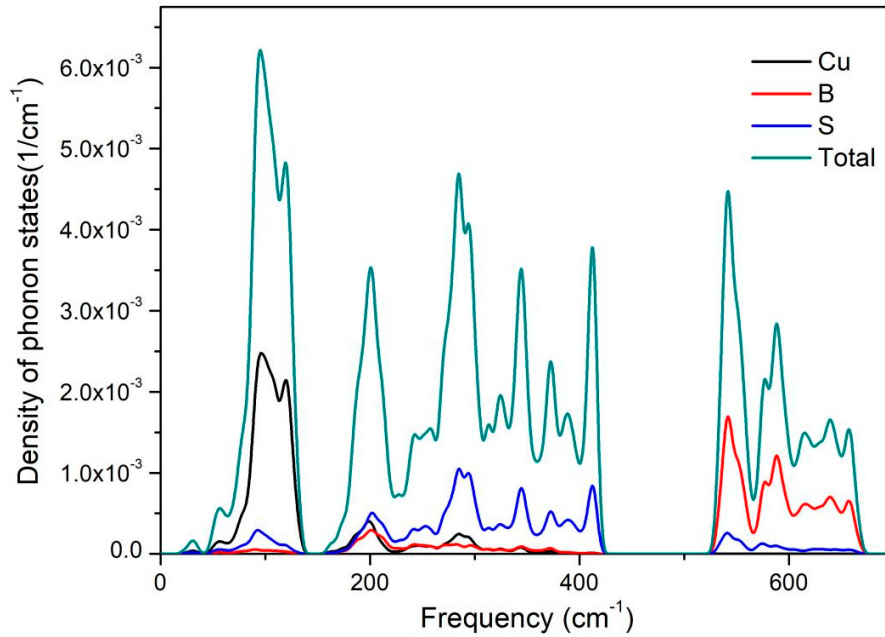


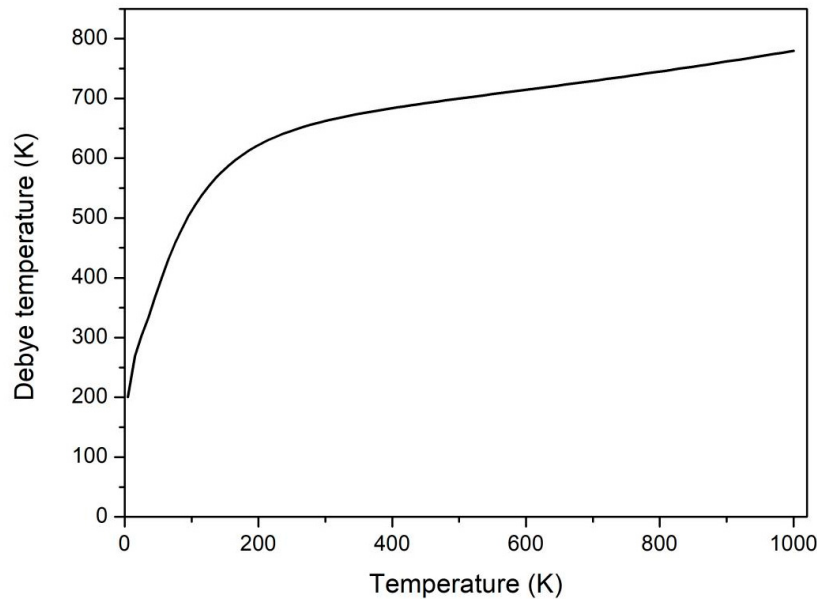
Figure 6: Phonon density of states (PDOS) of CuBS₂.

Table 3: Phonon frequencies of optical modes (unit in cm^{-1}) at the Γ point of CuBS_2 .

Modes	Activity	CuBS_2		Modes	Activity	CuBS_2	
		Present	Theo. [9]			Present	Theo. [9]
E	(IR, R)	619.68	660.856/686.354	B_1	(R)	595.948	636.04
E	(IR, R)	540.84	595.888/598.245	B_1	(R)	376.45	387.112
E	(IR, R)	330.9	342.992/343.093	B_1	(R)	120.09	132.789
E	(IR, R)	298.6	321.621/322.139	A_2	(S)	341.5	359.9
E	(IR, R)	191.94	217.131/218.149	A_2	(S)	415.63	429
E	(IR, R)	93.94	107.951/108.05	A_1	(R)	360.76	377
B_2	(IR, R)	159.48	178.803/178.872				
B_2	(IR, R)	344.4	357.832/360.12				
B_2	(IR, R)	532.67	579.771/619.75				

3.4 Thermodynamic Properties

Based on the calculated results of the phonon density of states, we employed the quasi-harmonic Debye model to compute the Debye temperature Θ_D of CuBS_2 , along with the temperature dependence of the free energy, enthalpy, entropy, and heat capacity, within a temperature range of 0–1000 K. Fig. 7 depicts the Debye temperature curve of the CuBS_2 crystal calculated in this study. It can be noted that in the low-temperature region (0–100 K), the Debye temperature increases sharply. After surpassing 100 K, the increase in the Debye temperature tends to level off. In the high-temperature region, the Debye temperature stabilizes around 760 K. Unfortunately, there are no experimental values for the Debye temperature of CuBS_2 crystal. For comparison, we examine the Debye temperature $\Theta_D = 284.9$ K [26] of chalcopyrite crystal CuInS_2 , it is large than the Debye temperature Θ_D of CuBS_2 in the 0 K.

**Figure 7:** Temperature-dependent Debye temperature of CuBS_2 .

As illustrated in Fig. 8, the free energy of the CuBS_2 crystal material exhibits a monotonic decrease with increasing temperature, while the enthalpy demonstrates a monotonic increase with rising temperature. Entropy, which defines the degree of disorder in a system, increases with rising temperature due to the

enhanced lattice vibrations in the CuBS_2 material. The trend in the product of temperature and entropy (TS), as illustrated in Fig. 8, further substantiates this conclusion.

As illustrated in Fig. 9, under low-temperature conditions, the specific heat capacity (C_v) of the CuBS_2 crystal exhibits a nearly proportional relationship with the cube of the temperature (T^3), thereby aligning with the Debye (T^3) law. Within the temperature range of 200 K to 500 K, the growth rate of specific heat capacity gradually decelerates. It can be found that specific heat capacity converges to a constant value at elevated temperatures, which aligns with the predictions of the classical Dulong–Petit law. This phenomenon indicates the reasonableness and reliability of the computational results presented in this study.

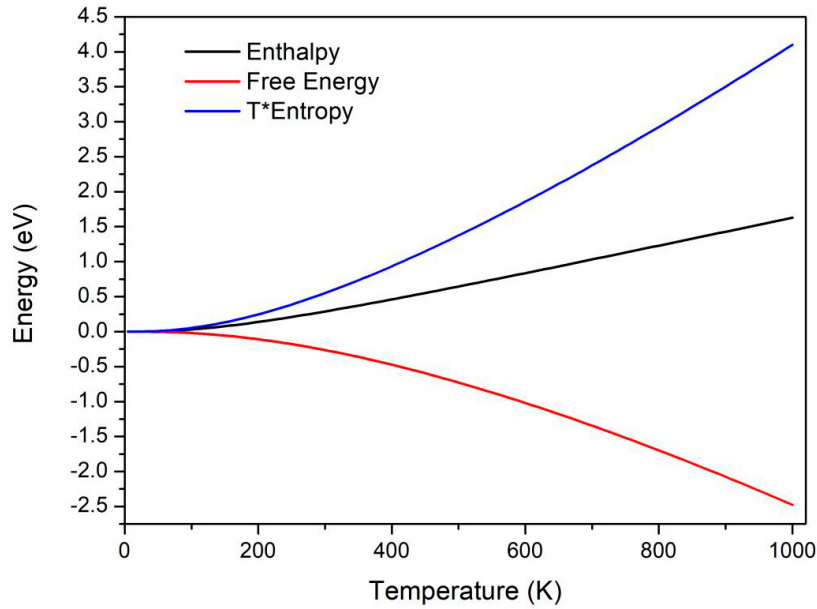


Figure 8: Temperature-dependent entropy, enthalpy, and free energy of CuBS_2 .

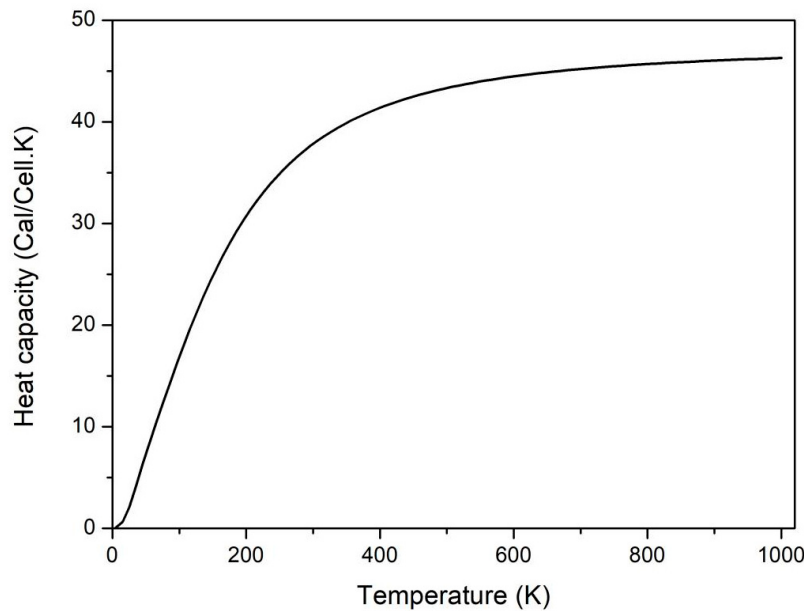


Figure 9: Temperature-dependent heat capacity of CuBS_2 .

4 Conclusion

In summary, the structural, elastic, lattice-dynamic, and thermodynamic properties of CuBS₂ have been studied using the first-principles method. The calculated lattice parameters are in excellent agreement with previous results. The results of elastic constants and phonon spectra indicate that CuBS₂ possesses both mechanical and dynamic stability. By analyzing the three-dimensional and two-dimensional plots of the elastic parameters, we found that this material exhibits significant elastic anisotropy. The calculated elastic anisotropy index and shear anisotropy factor of CuBS₂ indicates that the material has strong anisotropy and ductility. Finally, the thermodynamic properties, including the Helmholtz free energy, internal energy, specific heat, and entropy of CuBS₂, are determined.

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Author Contributions: The authors confirm contribution to the paper as follows: study conception and design: Dezi Li, Shunru Zhang; data collection: Dezi Li; analysis and interpretation of results: Dezi Li, Linhua Xie, Shunru Zhang; draft manuscript preparation: Dezi Li, Shunru Zhang. All authors reviewed and approved the final version of the manuscript.

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Conflicts of Interest: The authors declare no conflicts of interest.

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