First-principles calculation of the electronic structure, optical, elastic and thermodynamic properties of cubic perovskite LiBeF₃

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Abstract
The elastic, electronic structure, optical and thermodynamic properties of cubic fluoroperovskite crystal LiBeF₃ were investigated using the ab initio method. The calculated lattice parameter, elastic constants Cᵢⱼ, bulk modulus B and shear modulus G at 0 GPa and 0 K are agreed well with previous reports. The obtained band structure shows that LiBeF₃ has an indirect energy band gap of 7.64 eV, which is consistent with the known results. Then, the dielectric function, absorption coefficient, and refractive index were investigated. It was found that the absorption part of LiBeF₃ is located at the ultraviolet-light region. Finally, the thermodynamic properties of LiBeF₃, including the bulk modulus B, relative volume, heat capacities, thermal expansion α and relative Debye temperature at various temperatures and pressures, are discussed. The optical and thermodynamic properties, and their relationships of cubic crystal LiBeF₃ are reported for the first time. Our results indicate that LiBeF₃ compound is a promising optoelectronic and optics applications.

1. Introduction
In recent years, perovskite crystals have received widespread attention because of their application prospects in optical coatings, lens materials, semiconductor industry, photovoltaic applications and optoelectronic devices [1, 2], etc. The ternary fluoride compound ABF₃ with wider band gap is a common perovskite structure, where the cations A is alkali and B stands for alkaline earth metals. The group of fluoroperovskites crystals such as the LiBeF₃ crystal is excellent optical materials [3], such as the absence of optical anisotropy, low phonon energy and absorption and wide energy gap in the vacuum ultraviolet region. The LiBeF₃ crystal can be applied in a variety of photovoltaics, fuel cells, sensors and microelectronics, and it is also a promising material for memory devices [4, 5].

Nishimatsuet[1] found that the LiBeF₃ crystal has a wide energy gap, which is useful for a vacuum-ultraviolet-transparent lens material. Syrotuyk and Shved [6] investigated the electronic energy bands of the LiBeF₃ crystal within the LDA and GW formalism and revealed the existence of an indirect energy gap. Benmhidi [7] applied ab initio method with the FP-LMTO method to reveal the transport properties and calculated the indirect band-gap of LiBeF₃ as 7.83 eV. However, there is no experiment report about LiBeF₃ up to now because of there are some toxic materials during the synthesize process.

Therefore, in this work, we performed the structural, elastic, electronic, optical and thermodynamic properties investigations of the cubic LiBeF₃ crystal using the pseudo-potential plane-wave (PP-PW) method density functional theory (DFT) method. As far as we know, the reported theoretical investigations are mainly focused on the elastic and transport properties of cubic perovskite LiBeF₃ compound, while the optical, thermodynamic properties and their relationships of cubic LiBeF₃ have not been investigated yet.
2. Computational method

In the present work, the elasticity, thermodynamics and optical properties of the LiBeF3 crystal were investigated using PP-PW DFT in CASTEP software [8]. We used the local density approximation (LDA) [9] method with the Ceperley–Alder–Perdew–Zunger (CA–PZ) [10] functional, and the generalized gradient approximation (GGA) with the revised approximation of the Perdew-Burke-Ernzerh (PBE) [11] of scheme for the exchange-correlation potential. The ultrasoft pseudopotential was adopted to describe the interaction between particles. The valence electrons of Li atoms are 2s1, Be atoms are 2 s2, and F are 2s22p5. Meanwhile, screened exchange local density approximation (sX-LDA) [9] with non-conserving pseudopotential were implemented to calculate the value of energy band gap. The energy plane-wave basis energy cutoff was chosen to be 650 eV. The Monkhorst-Pack method was used to integrate the special k points into the Brillouin zone (BZ) sampling, with k-point mesh of 12 × 12 × 12 for the crystal structure optimization. The self-consistent convergence parameters were set as follows: total energy tolerance, SCF tolerance, maximum force tolerance, maximum stress and maximum displacement were taken as 5.0 × 10⁻⁶ eV/atom, 5.0 × 10⁻⁷ eV/atom and 0.01 eV/Å, 0.02 GPa and 5.0 × 10⁻⁴Å, respectively. These parameters were obtained based on the convergence tests. The Broyden–Fletcher–Goldforb–Shanno algorithm was used to optimize the geometric structure of LiBeF3, which helps us find the lowest energy structure. GIBBS program is used to evaluate the thermal properties of the material [12]. The space group of the cubic LiBeF3 crystal under normal temperature and pressure is Pm-3m. The Li atoms sitting at (0, 0, 0), the Be atoms at (1/2, 1/2, 1/2), and the three fluorine atoms at (1/2, 1/2, 0), (1/2, 0, 1/2), and (0, 1/2, 1/2), as shown in figure 1.

To investigate the thermodynamic properties of LiBeF3 crystal, the quasi-harmonic Debye model were applied. When the pressure and temperature are given, the non-equilibrium Gibbs function G*(V; P, T) is expressed as

\[ G^*(V; P, T) = E(V) + PV + A_{vib}(\Theta(V); T) \]

where \( E(V) \) represents the total energy per unit cell. \( A_{vib} \) refers to the Helmholtz free energy of vibration [13], which can be written as

\[ A_{vib}(\Theta; T) = nk_bT \left[ \frac{9\Theta}{8T} + 3\ln(1 - e^{-\Theta/T}) - D(\Theta/T) \right] \]

where \( \Theta \) represents the Debye temperature, \( k_b \) is the Boltzmann constant, \( n \) is the number of atoms per molecular unit. Poisson’s ratio is 0.25 for an isotropic solid. The Debye temperature [14] is written as

\[ \Theta = \frac{\hbar}{k_b} \left[ 6\pi^2V^{1/3}n^{1/3}f(\sigma) \right]^{1/3} \]

where \( M \) is the molecular mass per unit cell, \( f(\sigma) \) is given in the literature [15, 16], and \( B_S \) is approximated given by the static compressibility, which represents the adiabatic bulk modulus

\[ B_S \approx B(V) = V \left( \frac{d^2E(V)}{dV^2} \right) \]
Therefore, for a given condition (P, T), the unbalanced Gibbs free energy is only a function of volume. According to the minimized Gibbs function, we can calculate the equilibrium state in this state, which is

\[
\left( \frac{\partial G^*(V; P, T)}{\partial V} \right)_{P,T} = 0
\]  

(5)

By solving equation (5) [17], we will get the chemical potential and the thermal equation-of-state (EOS). The isothermal bulk modulus \( B_T \), the heat capacity \( C_v \), and the thermal expansion coefficient \( \alpha \) are expressed as

\[
B_T(P, T) = -V \left( \frac{\partial P}{\partial V} \right)_T
\]

(6)

\[
C_v = 3nk \left[ 4D \left( \frac{\theta}{T} \right)^2 - \frac{3\theta/T}{e^{\theta/T} - 1} \right]
\]

(7)

\[
\alpha = \frac{\gamma C_v}{B_T V}
\]

(8)

respectively, where \( \gamma \) is the Grüneisen parameter which can be written as

\[
\gamma = -\frac{d \ln \theta(V)}{d \ln V}
\]

(9)

3. Results and discussion

3.1. Elastic properties

The elastic constants \( C_{ij} \) describe the ability of deformation within a certain range of stresses on the material. The dynamical and mechanical responses of a compound under the applied stress are determined by Elastic constants [18]. Elastic modulus represent the response of material to the corresponding strain, which are obtained from elastic constants calculations. Many physical properties, such as development of crystal plastic deformation, enhanced charged defect mobility, mechanical yield points, elastic instability and phase transformations, are all affected by the elastic anisotropy [19]. For cubic crystals, the elastic constant \( C_{ij} \) has three non-zero independent components, namely \( C_{11}, C_{12}, \) and \( C_{44} \). Bulk and shear modulus \( B \) and \( G \) can be approximated by Voigt–Reuss–Hill (VHR). According to Voigt approximation [20] and Reuss approximation [21]

\[
G_V = \frac{C_{11} - C_{12} + 3C_{44}}{5}
\]

(10)

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

(11)

Hill theoretically proved that the polycrystalline modulus should be the arithmetic mean of \( G_V \) and \( G_R \):

\[
G = \frac{G_V + G_R}{2}
\]

(12)

When \( P \) is 0 GPa, the relation between \( C_{ij} \) and \( B \) of a cubic crystal is

\[
B = \frac{C_{11} + 2C_{12}}{3}
\]

(13)

For cubic crystals, mechanical stability conditions require elastic constants and satisfaction of the following three conditions [22]:

\[
\begin{align*}
\dot{C}_{44} & > 0, \\
\dot{C}_{11} & > |\dot{C}_{12}|, \\
C_{11} + 2\dot{C}_{12} & > 0
\end{align*}
\]

(14)

Because \( C_{11} > B > C_{12} \), the following relationship was established

\[
\dot{C}_{\alpha\alpha} = C_{\alpha\alpha} - p(\alpha = 1, 4)
\]

(15)

\[
\dot{C}_{ij} = C_{ij} + p
\]

(16)

In the present study, LDA and GGA were adopted to optimize the geometric structure of the LiBeF3 crystal cell, and the lattice constant \( a_0 \), elastic constant \( C_{ij} \), bulk modulus \( B_0 \), and shear modulus \( G \) under zero temperature and zero pressure were calculated. The results are tabulated and compared with previous works, as shown in table 1. As we can see, our results are in good agreement with the values of reference, which confirmed our calculations are believable.
where \( V \) refers to the volume of the unit cell, which is the equation for the energy operator, and \( \varepsilon \) is the momentum operator with \( i \) representing the QP energies without the effect of self-energy operator, \( \vec{p}_i \) is the momentum operator with \( i = x, y, z \), and \( \hbar \omega \) is the energy of the incident photon.

The absorption coefficient \( \alpha(\omega) \) can be obtained from the dielectric function. It is expressed as \( \alpha(\omega) = \sqrt{2} \omega [\sqrt{\varepsilon^2(\omega) + \varepsilon^2(\omega)} - \varepsilon(\omega)]^{1/2} \) (19)

The complex refractive index \( N(\omega) \) is represented as follows

\[
N(\omega) = n(\omega) + ik(\omega)
\]

where \( n(\omega) \) is the refractive index and \( k(\omega) \) represent the extinction coefficient.

### 3.2. Electronic structure

As shown in figure 2(a), the band structure of LiBeF\(_3\) is investigated. LiBeF\(_3\) is an indirect energy gap compound as the minimum value of the conduction band is located at the G point, and the maximum value of the valence band is located at the R point. The calculated energy gap is 7.26 eV, which is consistent with 7.73 eV [1] and 7.83 eV [7], respectively. These results show a wide band-gap for the LiBeF\(_3\) crystal. It can be seen that there is a discrepancy between this calculation and previously reported results. This is mainly because the LDA does not consider the discontinuity of the exchange-correlation potential between electrons, and the correlation effect between excited electrons in the multi-particle system is underestimated. Therefore, we applied sX-LDA and GGA-PBE function to calculate the band gap of LiBeF\(_3\) for comparison. The obtained values are listed in table 2. It can be found that sX-LDA results are more close to the previous results.

To obtain a more comprehensive diagram of the electronic structure, the results of the density of states (DOS) of LiBeF\(_3\) are represented in figure 2(b). According to figure 2(b), the valence band between \(-22.0\) and \(-19.0\) eV are dominated by F 2s states with minor contributions from Be 2s and 2p states, and the peak strength is 5.78 states/eV. The valence band between \(-7.18\) and \(0\) eV is mainly formed by F 2p with minor contributions from Be 2s and 2p, whose state density peak is located at \(-1\) eV. The conduction band is contributed by the hybrid of Be 2s and 2p and Li 2s states.

### 3.3. Optical properties

In this subsection, we investigated the optical properties of cubic perovskite LiBeF\(_3\). The complex dielectric function \( \varepsilon(\omega) \) is important for us to explore the optical properties of LiBeF\(_3\). According to the complex dielectric function one can calculate other spectra such as absorption coefficient \( \alpha(\omega) \) and complex refractive index \( N(\omega) \) [25]. It is written as [26]

\[
\varepsilon = \varepsilon_1 + i\varepsilon_2
\]

where \( \varepsilon_1(\omega) \) represent the real part and \( \varepsilon_2(\omega) \) is the imaginary part. From the electronic band structure of a solid, we can calculated \( \varepsilon_2(\omega) \), which is expressed as [27]

\[
\varepsilon_2(\omega) = \frac{4\pi^2\hbar^2}{m^2\omega^2V} \sum_{\nu,\nu',k} |\langle \nu' | \vec{p} | \nu \rangle|^2 \delta(E_{\nu'} - E_{\nu} - \hbar\omega)
\]

(18)

where \( V \) refers to the volume of the unit cell, \( E_{\nu'} \) and \( E_{\nu} \) represent the QP energies without the effect of self-energy operator, \( \vec{p}_i \) is the momentum operator with \( i = x, y, z \), and \( \hbar\omega \) is the energy of the incident photon.

The absorption coefficient \( \alpha(\omega) \) can be obtained from the dielectric function. It is expressed as [28]

\[
\alpha(\omega) = \sqrt{2} \omega [\sqrt{\varepsilon^2(\omega) + \varepsilon^2(\omega)} - \varepsilon(\omega)]^{1/2}
\]

The complex refractive index \( N(\omega) \) is represented as follows

\[
N(\omega) = n(\omega) + ik(\omega)
\]

where \( n(\omega) \) is the refractive index and \( k(\omega) \) represent the extinction coefficient.

### Table 1. Calculated lattice constant \( a_0 \), elastic constants \( C_{ij} \), bulk modulus \( B_0 \) and shear modulus \( G \) (GPa) under 0 GPa for the LiBeF\(_3\) crystal.

|          | \( a_0[\text{Å}] \) | \( B_0[\text{GPa}] \) | \( C_{11}[\text{GPa}] \) | \( C_{12}[\text{GPa}] \) | \( C_{13}[\text{GPa}] \) | \( C_{44}[\text{GPa}] \) | \( G[\text{GPa}] \) |
|----------|------------------|------------------|------------------|------------------|------------------|------------------|--------------|
| This work | 3.466            | 119.05           | 179.73           | 88.70            | 75.02            | 61.40            |              |
| LDA      | 3.515            | 111.64           | 162.35           | 86.28            | 72.00            | 56.29            |              |
| GGA      | 3.482            | —                | —                | —                | —                | —                |              |
| [23]     | 3.424            | 117.88           | 176.26           | 88.67            | 74.52            | 60.21            |              |
| [7]      |                  |                  |                  |                  |                  |                  |              |

The obtained \( C_{0} \) obey the cubic stability conditions, which can be expressed as \( C_{12} < B_0 < C_{11} \). According to the stability requirements of the cubic crystal structure, it can be found that the mechanical structure of the LiBeF\(_3\) crystal is stable in the given temperature and pressure. According to Pugh’s standard for crystal mechanics behavior [24], the quotient of \( B \) and \( G \) indicates the ductility of the crystal. Therefore, a low \( B/G \) value indicates that the material represents brittleness, and a high value shows ductility, and 1.75 is the critical value. It is calculated from the data in table 1 that the \( B/G \) value of LiBeF\(_3\) is 1.94, indicating that the LiBeF\(_3\) crystal can be classified as a slightly ductile material. The anisotropy factor can be accepted based on the equation:

\[
A = 2C_{44} / \left( C_{11} - C_{12} \right)
\]

When \( A = 1 \), the material shows completely isotropic. When the value of anisotropy factor is deviated from 1, this material shows an anisotropic property. In our result, we find the values of \( A \) for LiBeF\(_3\) is 1.65 and 1.92 by LDA and GGA function, indicating that LiBeF\(_3\) compound is an anisotropic material.

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**Note:** The table content seems to be a bit out of context from the main text. It likely represents calculated values for elastic constants and bulk modulus, but the mention of LDA and GGA standards is not fully contextualized within the provided paragraphs. The table might be intended to compare LDA and GGA results with previously reported data, indicating a comparison to literature sources such as [23] and [7].
The spectrum is generated by the transition between the conduction band and the valence band. The dielectric function \( \varepsilon(\omega) \) reflects the energy band structure and various other spectral information. Combined with the band structure and DOS, we can explain the peak value of the dielectric function. Figure 3(a) shows the relationship between the calculated imaginary part \( \varepsilon_2 \) and photon energy. It should be noted that the first critical points of the imaginary part \( \varepsilon_2 \) is located at 7.16 eV, which corresponds to the threshold for direct optical transitions between the conduction-band minimum (CBM) and the valence-band maximum (VBM). For

\[
\begin{align}
\varepsilon(\omega) &= \frac{\sqrt{\varepsilon_1^2(\omega) + \varepsilon_2^2(\omega)} + \varepsilon_1(\omega)}{2}^{1/2} \\
k(\omega) &= \frac{\sqrt{\varepsilon_1^2(\omega) + \varepsilon_2^2(\omega)} - \varepsilon_1(\omega)}{2}^{1/2}
\end{align}
\]

Table 2. Calculated energy gap values of LiBeF₃ using different exchange-correlation function.

| Function         | LDA-CA-PZ | GGA-PBE | sX-LDA | LDA   | LDA   |
|------------------|-----------|---------|--------|-------|-------|
| \( Eg(\text{eV}) \) | 7.26      | 7.27    | 7.64   | 7.73  | 7.83  |

\(^a\) [1].
\(^b\) [7].

Figure 2. (a) Calculated band structure and (b) density of states of the LiBeF₃ crystal.
LiBeF$_3$, the imaginary part $\varepsilon_2$ has four distinct peaks are located at 11.1 eV, 12.5 eV, 15.6 eV and 17.21 eV, corresponding to four absorption peaks in the absorption spectrum. The main peak is located at 15.6 eV, which corresponds to the intrinsic plasma frequency. The peak is attributed to the electronic transition from the F 2p states in the valence band to the Be 2p states in the conduction band. Combined with the PDOS, we can see that the band transition between 7.6 and 17.5 eV is generated by the excitation of electrons of Be 2s and 2p and Li 2s states.

The absorption coefficient of LiBeF$_3$ is shown in figure 3(b). We can see that the absorption part of LiBeF$_3$ is located at the ultraviolet range. It is noted that the major absorption edge begins at 7.31 eV, corresponding to the energy gap, which is originated from the electronic transitions from the F 2p states at the valence band to the Be 2p states in the conduction band. Combined with the PDOS, we can see that the band transition between 7.6 and 17.5 eV is generated by the excitation of electrons of Be 2s and 2p and Li 2s states.

The absorption coefficient $\alpha(\omega)$ of LiBeF$_3$ is shown in figure 3(b). We can see that the absorption part of LiBeF$_3$ is located at the ultraviolet range. It is noted that the major absorption edge begins at 7.31 eV, corresponding to the energy gap, which is originated from the electronic transitions from the F 2p states at the valence band to the Be 2p states at the conduction band. We note that the maximum absorption coefficient is at 18.2 eV. Compared with figure 3(a), the four absorption peaks completely correspond to the four dielectric peaks, which are the macroscopic representations of the transitions of solid electrons between the bands under the action of the photoelectric field wave perturbation. That is to say their transition mechanism is consistent.

The complex refractive index $N(\omega)$ of LiBeF$_3$ is shown in figure 4. We note that at 9.24 eV, the maximum value of the refractive index $n(\omega)$ is 1.7. The static refractive index $n(0)$ is calculated to be 1.37 for LiBeF$_3$. Both the extinction coefficient $k$ and the absorption coefficient $\alpha$ indicated that the absorption of light by the substance and the relationship between them can be expressed as $\alpha = \frac{2\pi k}{\lambda}$, where $\lambda$ is the wavelength. Namely, the peaks of extinction coefficient $k$ completely correspond to absorption peaks. The local maximum of $k(\omega)$ that corresponds to the zero of $\varepsilon_1(\omega)$ is 1.07 at 16 eV. The refractive index of the LiBeF$_3$ crystal shows obvious
brieffringence in the whole energy range, and the extinction coefficient shows strong anisotropy at the edge of the band. The reason is that the LiBeF$_3$ crystal belongs to the cubic system.

3.4. Thermodynamic properties
We investigated the thermodynamic properties of LiBeF$_3$ when temperature ranges from 0 to 1000 K and in the pressure range of 0–30 GPa, where the quasi-harmonic Debye model remains valid. We calculated the total energy and the corresponding volume $V$ of LiBeF$_3$. The variation of the total energies versus volume was fitted by the Birch–Murnaghan EOS [30], as shown in figure 5. The minimum value of the curve indicates the equilibrium volume $V_0$ and the zero-point energy of LiBeF$_3$, which were calculated to be $-81.1697$ Ha and 281.042 Bohr$^3$, respectively.

The bulk modulus $B$ of the crystal reflects the resistance of the material to external uniform compression under elastic systems. It is related to inter-atomic potentials. The bulk modulus $B$ of LiBeF$_3$ as a function of temperatures at various pressure are shown in figure 6. It can be found that bulk modulus nearly remains constant between 0 and 200 K. The bulk modulus decreases linearly with the elevated temperature when $T > 200$ K. When pressure $P$ is given, bulk modulus decreases with the elevated temperature $T$. Meanwhile, bulk modulus increases with the pressure $P$ decreasing when temperature is given. In figure 7, the functional image of the relative volume $V/V_0$ versus $P$ at different temperatures is presented. While temperature $T$ is given,
V/V₀ decreases with the increasing pressure. It is noted that V/V₀ of lower temperature is more than that of higher temperature at the same pressure P. This is because the increase of energy of particles at high temperatures, which leads to the increase of thermal motion and the solids are more easily compressed. In other words, increasing temperature has the same effect as increasing pressure on LiBeF₃.

In figure 8, CV and CP of LiBeF₃ are plotted for 0, 10, 20 and 30 GPa. At the same temperature, both CV and CP decrease with the increase of pressure. As presented in figure 8, the CV and CP curves are initially sharply increased, but their growth rate of curve gradually decreases. At relatively low temperatures, the vibrational excitations is only caused by acoustic vibrations, CV is proportional to T³, which is because the long-wavelength acoustical phonons are effective in this temperature range. The curve of CV inclines to approach the Dulong–Petie limit (124.75 J mol⁻¹k⁻¹) [31] at higher temperatures, this is due to the anharmonic effect of the crystal. Similarly, we can deduce that the increasing temperature and decreasing pressure have the same effect on heat capacity.

It is known that the thermal expansion coefficient α can directly reflect the structural stability of the material. Figure 9 shows the relationships between the thermal expansion coefficient α and temperature at different pressure. As shown in figure 9, α rapidly increases with the increasing temperature T at lower temperatures (T < 500 K), the increment of thermal expansion coefficient gradually slows down at higher temperatures, thus indicating that the LiBeF₃ crystal has good volume invariance at high temperatures. Meanwhile, α decreases with increasing pressure P when temperature is given, indicating that the LiBeF₃ crystal has good volume invariance at high pressure. That imply that the pressure increase can counteract the effect of the temperature increase on thermal expansion coefficient.

In figure 10, the variation of the relative heat capacity and Debye temperature versus pressure P when temperatures are 300, 600, and 1000 K for LiBeF₃ is presented. The dependences of the relative heat capacity and the relative Debye temperature on pressure are almost linear, but they have the opposite effects. The relative CV

![Figure 7. The relationships between relative volume V/V₀ and pressures at different temperatures for LiBeF₃.](image)

![Figure 8. Variation of the heat capacities CV (a) and CP (b) with temperatures at different pressures amounts.](image)
decreases with the increase of pressure, and the relative Debye temperature increases with the increase of pressure. For a given pressure, both the relative CV and the relative Debye temperature increase with increasing temperature. These results indicate that increasing the pressure on LiBeF$_3$ has the same effect as decreasing the temperature on LiBeF$_3$. Meanwhile, we calculated the Debye temperature of LiBeF$_3$ crystal at normal temperature ($T = 300$ K) as 1104.08 K. This relatively high Debye temperature indicates that the LiBeF$_3$ compound possesses excellent thermal conductivity.

4. Conclusions

Employing the density functional theory, we investigated the elastic, electronic structural, optical and thermodynamic properties of cubic perovskite LiBeF$_3$. The optical and thermodynamic properties of LiBeF$_3$ are reported for the first time. The calculated lattice constants $a$, bulk modulus $B$ and shear modulus $G$ at 0 GPa and 0 K are in consistent with previous results. The calculated electronic structure showed that the LiBeF$_3$ is an indirect band gap material with the energy band gap of 7.64 eV. Then, the absorption spectrum, dielectric function and complex refractive index were investigated. The absorption range of LiBeF$_3$ is found to be mainly
located in the range of ultraviolet-light region. The static refractive index is calculated to be 1.37. The local maximum of extinction coefficient $k(\omega)$ that corresponds to the zero of $\varepsilon_2(\omega)$ is approximately 1.07 at 16 eV for LiBeF$_3$. Through the quasi-harmonic Debye model, the dependence of the relative Debye temperature, thermal expansion parameter, relative volume, heat capacities at various temperatures and pressures, and trends are discussed. The calculated coefficient of thermal expansion $\alpha$ indicates that the LiBeF$_3$ compound has good volume invariance at high temperatures. The Debye temperature has also been investigated. Our results indicate the cubic perovskite LiBeF$_3$ is a promising optoelectronic and optics applications.

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