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Electronic and optical properties of the zinc-blende structured LiZnN under pressure*

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The electronic and optical properties of the cubic zinc-blende (ZB) structured filled tetrahedral semiconductor α-LiZnN under pressure are investigated by using *ab initio* plane wave pseudopotential density functional theory method within the generalized gradient approximation (GGA). The electronic band structure and the density of state under pressure are systematically described. The basic optical constants, including the reflection and absorption spectra, the energy-loss function, the complex refractive index and the dielectric function, are calculated and analysed at different external pressures. Our results suggested that the ZB α-LiZnN is transparent in the partially ultra-violet to the visible light region, and it seems that the transparency is hardly affected by the pressure.

Keywords: density functional theory, electronic structure, optical properties, LiZnN
PACC: 7115M, 7115H, 7865K

1. Introduction

The III–V compound semiconductors have been viewed as a promising system for the device applications in electronic and optoelectronic technologies.[1] In recent years, the binary analogue filled-tetrahedral compounds (FTCs) $A^{I}B^{II}C^{V}$ with (A^{I}=Li, Cu, Ag; B^{II}=Be, Mg, Zn, Cd; C^{V}=N, P, As, Sb, Bi) have been found to constitute an interesting family of semiconductors and have been extensively studied.[2−13] Especially, the FTC compounds LiZnX (X=N, P, As) have attracted great attention.[2−7] They are usually subjected to large built-in strain since they are often grown on different substrates having considerable lattice mismatch, also a difference in the thermal expansion coefficients between epitaxial layer and substrate.[4] The cubic zine-blende (ZB) structured filled-tetrahedral semiconductor compound LiZnX belongs to space group F-43m (No.216) which can be characterized as an 'empty tetrahedral interstitial structure', with its four lattice sites in unit cell, namely, $\tau_1 = (0,0,0)a_0$, $\tau_2 = (1/4,1/4,1/4)a_0$, $\tau_3 = (1/2,1/2,1/2)a_0$, $\tau_4 = (3/4,3/4,3/4)a_0$ (a_0 denotes the lattice parameter). The III–V compound semiconductors $D^{III}C^{V}$ have the D^{III} atom at τ_1 and the C^{V} atom at τ_2. One could transmute the D^{III} atom into its isovalent pair A^{I}+B^{II} atoms. The A^{I} atom can occupy either the τ_3 site (corresponding to the α phase) or the τ_4 site (corresponding to the β phase). The main feature of these compounds is the translation of the band structure from an indirect to a direct one in comparison with the binary III–V analogous compounds. Therefore, a detailed investigation of the dependence of electronic and optical properties on pressure is an important subject to study either from a fundamental or an application aspect.

The FTC compounds have aroused great scientific interest from many research groups in the world due to their interesting properties, such as, their structural transformation and bonding character.[14−20] The electronic band structure was calculated and interpreted by means of the insertion rule.[21] The electronic and optical properties of the FTC compounds under normal pressure were presented by Kalarasse *et al.*[4,10] The elastic properties have been investigated by Kalarasse and Bennecer[3] and Bouhemadou *et al.*[5] Yet, there are very few reports on the electronic and optical properties of this interesting semiconductor's family under high pressure (to our knowledge), although their promising potential technological applications have been emphasized. Until recently, the pressure effect on the optical properties of the filled tetrahedral semiconductors LiZnX (X=N, P, As) has been reported by Kalarasse *et al*,[2] who investigated them by using the full-potential linear aug-

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mented plane wave method (FP-LAPW). They conducted a comparative study among the compounds LiZnX (X=N, P, As) as well as GaX (X=N, P, As). However, it is well known that the optical properties are closely related to the electronic properties, and are reflected by the bond structure and the density of states. But Kalarasse *et al* [2−4] only gave a simple description of the band structure and optical properties of the compounds.

In this work, we focus on one member of the FTC compounds, LiZnN, and study it using a different method. The aim of this work is to give a detailed description of the bond characteristic, electronic band structure, density of states and optical properties of the ZB α-LiZnN compounds under high pressures. Here we apply the Cambridge Serial Total Energy Package (CASTEP) program within the frame of density function theory (DFT).[22,23] Applying this theory, we have recently investigated the elastic properties of some materials.[24,25] The rest of this paper is organized as follows. In Section 2, we briefly review the theoretical method. The detailed description and analysis of our results are presented in Section 3. Finally, a conclusion of the present study is given in Section 4.

2. Calculation method

2.1. Total energy electronic structure calculations

In all the electronic structure calculations we adopt the non-local pseudopotential introduced by Vanderbilt[26] for the interactions of the electrons with the ion cores, together with the generalized gradient approximation (GGA) for exchange-correlation functional in the scheme of Perdew–Burke–Ernzerhof (PBE).[27] In the present calculations, the electronic wave functions are expanded in a plane wave basis set with energy cut-off of 380 eV, pseudo-atom calculations are performed for Li ($1s^2 2s^1$), Zn ($3d^{10} 4s^2$) and N ($2s^2 2p^3$). The K-space integration has been performed using 8×8×8 k points in the irreducible Brillouin zone (IBZ), which ensures self-consistent convergence differences of the total energy within 5.0×10^{-7} eV/atom. These parameters are sufficient in leading to well converged total energy and geometrical configurations. All total energy electronic structure calculations are implemented through the CASTEP code.[22,23]

2.2. Optical properties

The linear optical properties in solids can be described with the complex frequency-dependent dielectric function $\varepsilon(\omega) = \varepsilon_1(\varepsilon) + \mathrm{i}\varepsilon_2(\omega)$. Since α-LiZnN compounds have cubic symmetry, we only need to calculate one dielectric tensor component to completely characterize the linear optical properties. The imaginary or absorptive part $\varepsilon_2(\varepsilon)$ of the frequency-dependent dielectric function is given by[28]

$$\varepsilon_2(\omega) = \frac{e^2\hbar}{\pi m^2\omega^2}\sum_{v,c}\int_{\mathrm{BZ}} |M_{cv}(\kappa)|^2 \delta\left[\omega_{cv}(k) - \omega\right] \mathrm{d}^3k. \tag{1}$$

The integral is carried out over the first Brillouin zone, and the momentum dipole elements $M_{vk}(k) = \langle u_{cv}|e\cdot\nabla|u_{ck}\rangle$, where e is the potential vector defining the electric field, are matrix elements for direct transitions between valence-band $u_{vk}(r)$ and conduction-band $u_{ck}(r)$ states, and the $h\omega_{cv}(k) = E_{ck} - E_{vk}$ is the corresponding transition energy.

The real part $\varepsilon_1(\varepsilon)$ of the frequency-dependent dielectric function can be derived from the imaginary part using the Kramers–Kronig relations

$$\varepsilon_1(\omega) = 1 + \frac{2}{\pi}p\int_0^\infty \frac{\omega'\varepsilon_2(\omega')}{\omega'^2 - \omega^2}\mathrm{d}\omega', \tag{2}$$

where P denotes the principal value of the integral. Based on the knowledge of both real and imaginary parts of the frequency-dependent dielectric function, we can calculate the important optical functions such as the refractive index $n(\omega)$

$$n(\omega) = \left[\frac{\varepsilon_1(\omega)}{2} + \frac{\sqrt{\varepsilon_1^2(\omega) + \varepsilon_2^2(\omega)}}{2}\right]^{1/2}. \tag{3}$$

In order to investigate the optical properties, a sufficiently dense k-mesh is used in the present work, which consists of 15×15×15 k-mesh.

3. Results and discussion

3.1. Electronic structures of ZB α-LiZnN under pressure

First of all, we carry out first-principles calculation to find the most stable structure of α-LiZnN. We set a series of different values of lattice constant a to calculate the total energy E and the corresponding primitive cell volume V for the ZB α-LiZnN. By fitting the calculated energy–volume ($E-V$) data to the third-order natural strain equation of states (EOS)[29]

$$P = 2B_0 \left(\frac{V_0}{V}\right) f_{\rm N} \left[1 + \frac{3}{2}\left(B' - 2\right) f_{\rm N} + \frac{3}{2}\left(1 + B^0 B'' + \left(B' - 2\right) + \left(B' - 2\right)^2\right) f_{\rm N}^2\right], \quad (4)$$

where $f_{\rm N} = \ln(l/l_0)$, which may be written as $f_{\rm N} = \ln(V/V_0)/3$ for hydrostatic compression. Through these calculations, we can obtain the equilibrium lattice constants a. In Table 1, the calculated lattice constants, charge transfer, bond lengths and bond populations of ZB α-LiZnN at different external pressures are presented. From this table we can see that our lattice constant for ZB α-LiZnN is consistent with the experimental data reported recently. And we also found that the lattice constant is decreased to about 5.4% of the initial value when the external pressure is increased from 0 to 30 GPa. Meanwhile, the absolute values of charge transfer are increased for the Li and Zn ions from 1.76 to 2.11 eV and from 0.70 to 1.11 eV, respectively. However, the bond lengths are reduced with increasing pressure. For the Li→N and N→Zn, the reductions are all from 2.133 to 2.018 Å; for the Li→Zn, the reduction is from 2.464 to 2.330 Å. And the absolute value of bond population is also enhanced when the ZB α-LiZnN is compressed from 0 to 30 GPa. Namely, for the Li→N, it is from 0.97 to 1.61 eV, for the N→Zn is from 2.89 to 3.61 eV, and for the Li→Zn is from 6.89 to 14.49 eV. In conclusion, it is noticed that the charge transfer and the bond population are increased but the bond length is reduced. This is easily understood for more electron clouds overlap together and more charges transfer among the Li, Zn and N atoms when the bond length is shortened under pressure.

Table 1. Calculated lattice constants, charge transfer, bond lengths and bond populations of ZB α-LiZnN at different external pressures.

pressure/GPa	lattice constant/Å	charge/eV			bond length/Å			bond population/eV		
		Li	Zn	N	Li–N	N–Zn	Li–Zn	Li–N	N–Zn	Li–Zn
0	4.927 4.91[a], 4.902[b]	1.76	–0.70	–1.06	2.133	2.133	2.464	–0.97	2.89	–6.89
5	4.863	1.83	–0.75	–1.08	2.106	2.106	2.432	–1.11	3.05	–7.81
10	4.828	1.87	–1.08	–0.79	2.091	2.091	2.414	–1.19	3.14	–8.46
15	4.758	1.96	–1.10	–0.86	2.060	2.060	2.379	–1.36	3.32	–10.24
20	4.734	1.99	–1.10	–0.98	2.050	2.050	2.367	–1.42	3.39	–11.06
25	4.677	2.08	–1.11	–0.97	2.025	2.025	2.339	–1.57	3.56	–11.37
30	4.660	2.11	–1.11	–0.99	2.018	2.018	2.330	–1.61	3.61	–14.49

* Here a and b denote the experimental values taken from Refs.[10] and [12] for α-LiZnN, respectively.

Since the FTC compounds with direct gap are promising materials for technological applications, and the electronic structures are closely related to the optical properties, in order to investigate the optical properties under pressure, it is interesting to know the dependence of electronic properties on pressure. For the ZB α-LiZnN, in Figs.1(a) and 1(b) are illustrated the calculated electronic band structure (left panel) and the total density of states (TDOS) (right panel) along the various symmetry lines at 0 GPa and 30 GPa, where the top of the valence band is taken to be zero energy. The overall band profiles are in good agreement with other theoretical results.[2] Namely, the valence bands are arbitrarily aligned and start from lower energy. In the present work, we take no account of the spin–orbit interaction. These figures show that the top of valence band and the bottom of the conduction band are all at the G-symmetry point, which indicates that the ZB structured FTC compound α-LiZnN has a direct gap. And we found that the direct band gap $G_{\rm v} - G_{\rm c}$ occurs at about 0.526 eV, which is very close to that in Ref.[7], and the smallest indirect band gap is 2.308 eV, which is consistent with that obtained by Kalarasse and Bennecer.[4] Furthermore, if we compare Fig.1(a) to Fig.1(b), we find that the valence band of ZB α-LiZnN shifts downwards, while the conduction band shifts upwards with increasing pressure. From the TDOS diagram we find that the TDOS at the edges of the band gap is small and the peaks of DOS descend with increasing pressure. In addition, the conduction and valence bands have a tendency to shift the higher and lower energies, respectively. In Table 2, we list the direct and indirect band gaps together with other theoretical results for the ZB α-LiZnN at different external pressures. From this table we find that these energy gaps are widened with elevated pressure; this exactly corresponds to the variation of band structure, i.e. the valence and conduction bands of ZB α-LiZnN shift downwards and upwards with

increasing pressure, respectively.

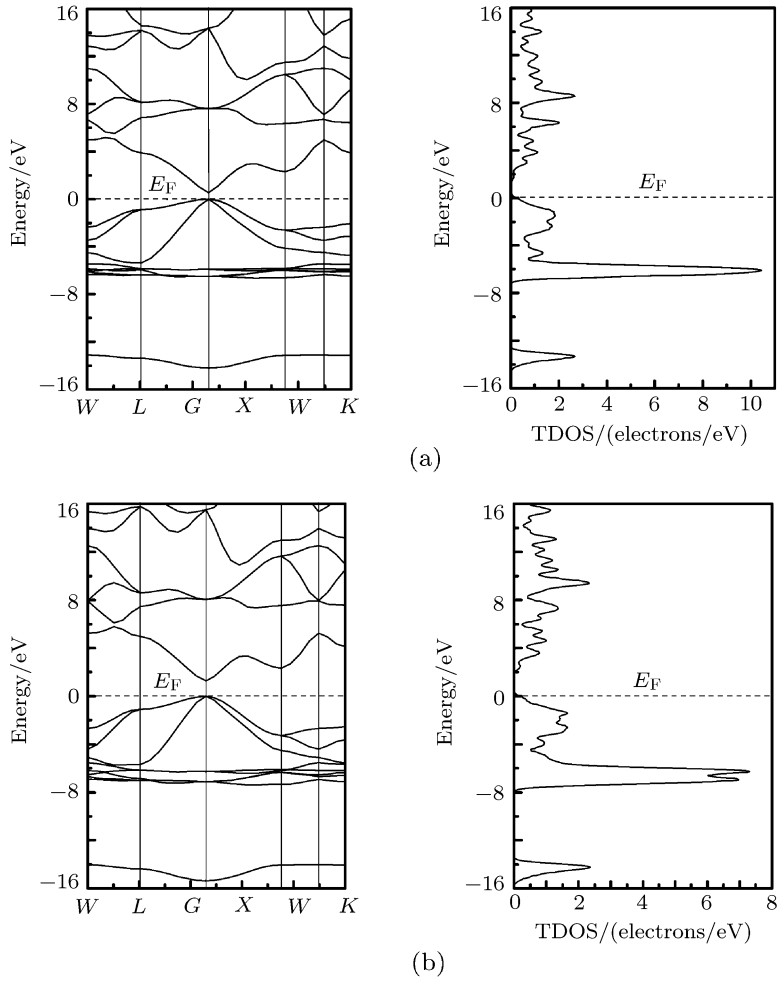


Fig.1. Band structure and total density of states (TDOS) for ZB α-LiZnN along the principal symmetry direction at 0 K: (a) 0 GPa, (b) 30 GPa.

Table 2. Calculated energy gaps E_g/eV of the ZB α-LiZnN for different pressures.

pressure/GPa	energy gaps/eV				
	$G_v - G_c$	$G_v - L_c$	$G_v - X_c$	$L_v - L_c$	$X_v - X_c$
0	0.526	3.899	2.308	4.781	4.927
	0.940,[4] 0.601,[7] 1.91[15]		2.29,[4] 2.34[7]		
5	0.699	4.135	2.318	5.063	5.070
10	0.795	4.267	2.323	5.223	5.157
15	0.993	4.544	2.334	5.556	5.338
20	1.064	4.642	2.338	5.673	5.403
25	1.231	4.879	2.347	5.960	5.562
30	1.281	4.951	2.350	6.047	5.611

In order to further investigate the effects of pressure on the electronic structures of the ZB α-LiZnN, the partial density of states (PDOS) for the ZB α-LiZnN at 0 GPa and 30 GPa are shown in Figs.2(a) and 2(b) respectively, from which we can see that the highest valence bands are essentially dominated by Zn

3d states, with a minor presence of N 2p states. The other valence bands are essentially dominated by N 2s states, with a minor presence of Zn 4s states. The conduction band consists mainly of Zn 4s and N 2p states. Our results for PDOS curves resemble those of the other theoretical work in Ref.[4]. In addition, the peaks of PDOS are descending (except that the DOS of Li is zero), for instance, for the Zn 3d orbital the obvious peaks are shifted from –6.06 to –6.28 eV, for the N 2s orbital the peak from –13.33 to –14.25 eV and for the N 2p orbital from –1.17 and –1.40 eV to –6.37 and –6.99 eV, respectively. But the bandwidth becomes broader approximately from 0.526 eV at 0 GPa to 1.281 eV at 30 GPa, which implies that the electrons in those states are active under pressure. This phenomenon corresponds to that in Figs.1(a) and 1(b), the low band consists of the group of N atom s states. The second narrow group of bands is mainly due to the Zn atom d states. However, the contribution of the N atom p state is small. The rest of the valence and conduction bands are a mixture of p and s states

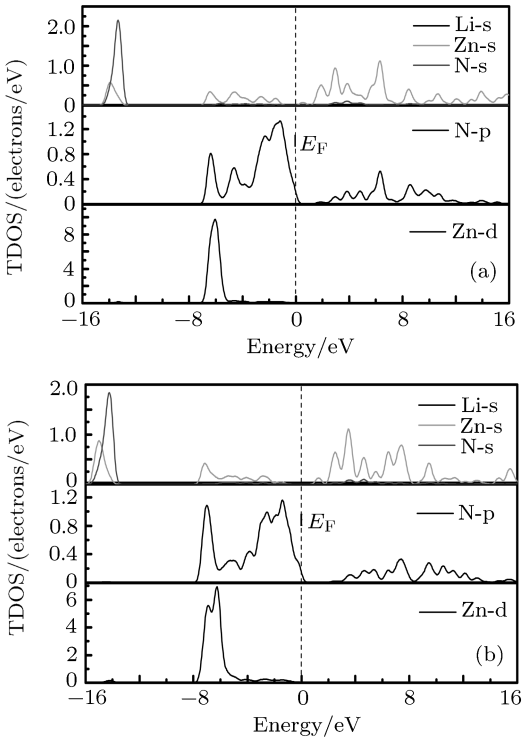


Fig.2. Partial density of state (PDOS) of the ZB α-LiZnN at 0 K: (a) 0 GPa, (b) 30 GPa.

with a small amount of d states (see Ref.[30] for more details).

From the band structures of ZB α-LiZnN, it is obvious that the upmost of the valence bands are flat, indicating that the compounds have large-hole effective masses, which should result in some unusual transport properties of the p-type semiconductor, as well as the change of the DOS and band structure hybridization under pressure; thus this kind of material may have some unusual optical properties and potential applications.[31] This is the main reason why we discuss the optical properties of ZB α-LiZnN under pressures in detail.

3.2. Optical properties of ZB α-LiZnN under pressure

In this subsection, we will discuss the frequency-dependent optical properties of the ZB structured FTC compounds α-LiZnN, and the influence of external pressure on the optical properties. The complex refractive index N is generally defined as $N(\omega) = n(\omega) + \mathrm{i}K(\omega)$, where the imaginary part $K(\omega)$ is related to the absorption coefficient by $\eta = 2k \cdot \omega/c$. While the complex dielectric constant is related to the complex refractive index by $\varepsilon(\omega) = \varepsilon_1(\varepsilon)+\mathrm{i}\varepsilon_2(\omega)$. And the reflectivity coefficient R is related to the complex refractive index by $R(\omega) = |(1-N)/1+N|^2$. In the present work, the optical properties including dielectric function, absorption, reflectivity and energy-loss function are calculated and analysed.

The absorption coefficient $\alpha(\omega)$ and the reflectivity coefficient $R(\omega)$ for the ZB structured FTC compounds α-LiZnN at different pressures are shown in Fig.3. It is not difficult to find the two remarkable peaks at about 10.5 and 14.7 eV, and there is almost no absorption at the lower energy region from about 0 to 2 eV. It means that the material is transparent in the partially ultra-violet to the visible light region because phonon energy at such a range is just within the forbidden band. The absorption occurs from about 2 to 35 eV at different pressures with a slight shift towards the high-energy region and the positions of the peaks are moved towards the higher energy direction with increasing pressure. For the reflectivity curve, the first or the strongest absorption peak takes place around 11.6 eV. However, at the high-energy region, where photon energy is larger than about 30 eV, the reflection is very weak and tends slowly to zero with increasing photon energy. Obviously, the corresponding relationship between the absorption and reflection spectra is that in the region where absorption is intense, the reflectivity is also larger. This means that if a material can strongly absorb light in some region, it can also effectively reflect the light in the same re-

gion. From comparison, it can be shown that the shape of the absorption coefficient curve is not sensitive to the pressure. However, the positions of the peaks are shifted towards the lower wavelength direction with increasing pressure.

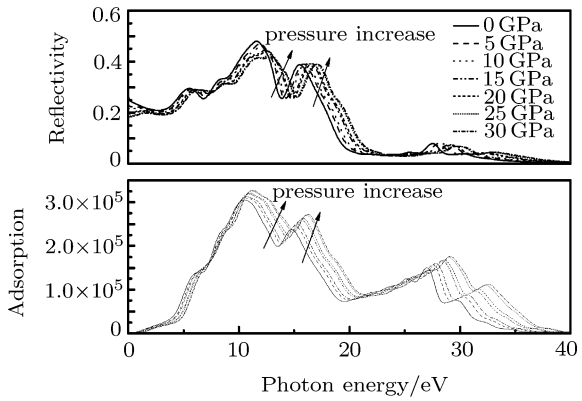


Fig.3. The absorption and reflectivity curves at different external pressures for ZB α-LiZnN.

The electron energy-loss spectra $L(\omega)$ at normal (solid line) and external pressure (dot-dashed) are shown in Fig.4. $L(\omega)$ describes the energy loss of a fast electron transferring in a material. From this figure we can see that there are two prominent peaks in $L(\omega)$ spectra which represent the characteristics associated with the plasma resonance. The positions of peaks in the $L(\omega)$ spectra also indicate the point of transition from metallic to dielectric property for a material. And there is a lossless region from 0 to about 5.0 eV. It is noticed that just the electron with energy less than 5.0 eV can be transmitted in ZB α-LiZnN.

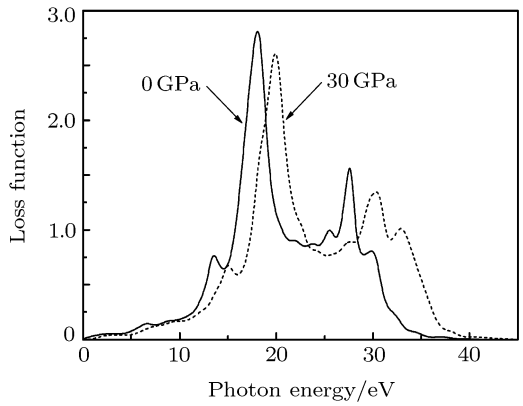


Fig.4. The loss function curves for ZB α-LiZnN at 0 GPa (solid curves) and 30 GPa (dashed curves).

In Fig.5, we display the real and imaginary parts of the complex refractive index $n(\omega)$ curves for the photon energy from 0 to 45 eV at different external pressures. Obviously, the sharp peaks mainly exist in the low energy region and the highest peak occurs at about 10.5 eV. This indicates that the line shape of the refractive index curve changes little with pressure, but the positions of the peaks move towards the higher energy direction. Moreover, the values of the imaginary part are very small, and the real part changes little in the high energy region (photon energy larger than 20 eV). The phenomena show that the absorption of high frequency electromagnetic waves is very weak, and the refractive index is almost constant in the high frequency region.

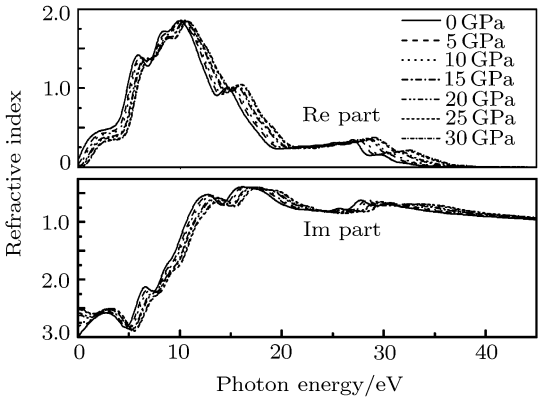


Fig.5. Refractive index curve at different external pressures for ZB α-LiZnN.

The real part $\varepsilon_1(\varepsilon)$ and the imaginary part $\varepsilon_2(\varepsilon)$ of the dielectric function of α-LiZnN under normal and high pressures are shown in Fig.6. We can observe that the line shapes of $\varepsilon_1(\varepsilon)$ and $\varepsilon_2(\varepsilon)$ are practically unchanged, while there is a little shift towards the high-energy region when the material is compressed from 0 to 30 GPa, which is consistent with the results in Ref.[2]. Since their origin in K space remains unchanged under pressure, the shifts of these peaks to higher energy are due to the increase of the band gaps. For the imaginary part $\varepsilon_2(\varepsilon)$, in the energy range of about 4.5–9.0 eV at ambient pressure, there are two peaks: the first is mainly due to the transition from the two highest valence bands to the lowest conduction band (as shown in Fig.1). Our analysis of the $\varepsilon_2(\varepsilon)$ curves show that the threshold energy "first critical points" of the dielectric function occurs at about 5.6 and 6.7 eV at 0 and 30 GPa, respectively. These points are $G_{\mathrm{v}} - G_{\mathrm{c}}$ splitting which gives the threshold for direct optical transitions between the highest valence band and the lowest conduction band. This is known as the fundamental absorption edge. In addition, according to the Kramers–Kronig dispersion relation, the real part $\varepsilon_1(\varepsilon)$ of the frequency-dependent dielectric function at 0 and 30 GPa is also obtained and

displayed in Fig.6. The main peaks for the real part $\varepsilon_1(\varepsilon)$ in the spectra are situated at 4.5 and 5.4 eV at 0 GPa and 30 GPa in the energy range from 0 to 18 eV, respectively. And the peaks for the imaginary part $\varepsilon_2(\varepsilon)$ are at about 5.5 and 6.7 eV, which are also

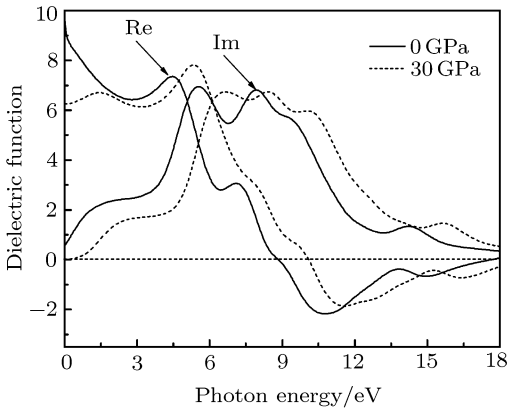


Fig.6. The real and imaginary parts of the dielectric function curves for ZB α-LiZnN at 0 GPa and 30 GPa.

similar to those in Ref.[2] on the whole. In conclusion, although the positions of these peaks are shifted under pressure, they are still of the same type as those at zero pressure. Moreover, the intensity of these main or global peaks is smaller but wider under pressure.

4. Conclusions

We have studied the electronic and optical properties of ZB α-LiZnN under pressure by means of *ab initio* pseudopotential density functional method. We found that the ZB structured filled-tetrahedral compounds α-LiZnN have direct gap and the dependence of energy gap on pressure has also been obtained. The optical coefficients are calculated for different pressures. The results show that it is transparent in the range from the near ultra-violet to the visible light region. Under external pressures, the blue shift of the absorption spectrum will occur, which is due to the broadening of the band gap, and the photon energy shifts towards high-energy region with increasing pressure.

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