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CaX (X=S, Se, Te)带隙的 GW 近似修正

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摘 要：采用基于第一性原理下的局域密度近似(LDA)方法对岩石矿物结构 Ca 硫族化合物 CaX (X=S, Se, Te)的晶格常数和电子结构进行了研究. 研究结果表明，使用 LDA 方法得到的晶格常数与实验值符合得很好，但带隙值却远低于实验值. 为了获得可靠的带隙值，使用了 GW(G 格林函数，W 库伦屏蔽相互作用)近似方法对 Ca 硫族化合物的带隙进行修正. 利用 GW 近似方法计算 CaS 和 CaSe 的带隙值比利用 LDA 计算的带隙值高，并且与实验值相吻合. 同时也预测了 CaTe 的带隙值，尽管没有实验值作为参考，但 GW 近似计算的结果应该是合适的值.

关键词：带隙；CaX (X=S, Se, Te)；GW 近似
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Band gaps of CaX (X=S, Se, Te) in GW approximation correction

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Abstract: The structures and electronic properties of calcium chalcogenides CaX (X=S, Se, Te) in NaCl structure have been investigated by using the first-principle pseudopotential method based on density function theory within a LDA (local density approximation). The calculated lattice parameters are in excellent agreement with the experimental results, whereas the minimum gaps are much lower than the experimental ones. To get the reliable band gap values, we employ the GW (G is Green's function and W is the screened Coulomb interaction) approximation method to correct the band gap values. The band gap values of CaS and CaSe using GW approximation have been improved compared to the obtained results from the LDA, which are in agreement with the experimental data. And we also predict the band gap value of the CaTe. It is expected that GW approximation should be very appropriate, though there is no experimental result for CaTe.

Keywords: Band gap; CaX (X=S, Se, Te); GW approximation

1 Introduction

The calcium chalcogenides CaX (X=S, Se, Te), like other alkaline-earth chalcogenides have attracted much attention from both experimental and theoretical points of view[1-8]. This is due to their wide applications in various technological fields, such as luminescent devices, radiation dosimetry, fast high-resolution optically stimulated luminescence imaging and infrared sensitive devices[9-12]. These applications require a complete understanding of the electronic properties of these

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materials, especially the band gap. The band gap values are simple but important parameter of semiconductor and insulator and also give important information about the electrical and optical properties of a solid. So, it is necessary to get the accurate band gap values of calcium chalcogenides in both theory and experiment. Shameen Baun *et al*. have investigated the electronic band structures of CaX (X=S, Se, Te) in NaCl structure, using the tight binding linear muffin-tin orbital within the local-density approximation. Their studies showed an indirect band gap (Γ−X) of 2. 36 eV for CaS, 1. 98 eV for CaSe and 1. 35 eV for CaTe, respectively[13]. The indirect band gap values (Γ−X) are 1. 9 and 2. 15 eV for CaS reported by Shaukat *et al*. Using the local-density approximation (LDA) and the Generalized Gradient approximation (GGA) respectively[3]. These calculations are much lower than experimental values (4. 434[5], 3. 5[12], and 4. 52[14] eV for CaS, 3. 85 and 3. 93[5] eV for CaSe[14]). Then the Hartree-Fock method has been applied to compute the electronic band structure by Pandey *et al*.[15], their investigations indicated that the band gap (Γ−Γ) of 7. 6 eV for CaS. But this band gap value is much higher than experimental values, and the results showed that CaS is direct band-gap semiconductor[15]. Although the result of the Labidi *et al*. by the Generalized Gradient approximation by Engel and Vosko (EVGGA) showed that significant improvement over other theoretical work, the minimum indirect band gap values are 3. 18 eV for CaS, 2. 81 eV for CaSe and 2. 23 eV for CaTe[8], which are still lower than the experimental values.

As everyone knows, calculations using LDA and GGA in density functional theory (DFT) are very reliable for structural parameters (error of few percent in the lattice constants, bulk modulus)[4, 8, 16-18]. However, LDA and GGA are not to be predictive for excited state properties. For some materials, their calculations usually underestimate the band gap values by about 30%～40%[7, 19, 20], while band gap values calculated using Hartree Fock (HF) method are 2～3 times larger than that of experimental values[21]. To overcome these problems and obtain the accurate band gap values, there are some pragmatic and relatively low-cost approximations as LDA+U, LDA-SIC (self-interaction correction), the screened exchange method and so on. But there are some limitations in correcting the band gap using the above methods. For the LDA+U, it depends on a parameter U, which is often adjusted to experiments[22], while the LDA-SIC did not very well in correcting the band gap[23].

In this work, we have considered the many-body effects using the GW (G is Green's function and W is the screened Coulomb interaction) approximation method of Hedin[24] to obtain the appropriate values of the band gaps, which has been successfully tested in semiconductors and insulators[25-29]. It was rarely used because its high computational costs. By virtue of recent advances in computational power and techniques, the GW approximation becomes common approach to estimate band gap. This paper presents the structures and band gap values of CaX (X=S, Se, Te) in NaCl structure under LDA and corrects the band gap values in the GW approximation.

2 Method

2.1 LDA

The calculations have been performed in a self-consistent manner using the ABINIT code[30]. An efficient fast Fourier transform algorithm[31] is used for the conversion of the wave functions between the real and the reciprocal lattices. The Kohn-Sham orbitals are expanded in a plane-wave basis set. We consider a non-local Troullier-Martins (TM) pseudopotential[32] within a separable approximation[33] generated by Fritz Haber Institute (FHI) code[34]. For the exchange-correlation functional, the LDA is employed[35-37]. To confirm the convergence of our calculations, we carefully investigate the dependence of the total energy on the cut off energy and the k-point. When the cutoff energy is fixed in

50.0 Hartree (1360.57 eV), the change in total energy is less than 0.24 meV when the k-point is beyond 4×4×4; on the other hand, when the k-point is fixed in 4×4×4, the convergence in total energy is very well when the cutoff energy is higher than 40.0 Hartree (1088.46 eV). In consideration of two criterions: (1) the interested special k-piont to determine the band gap should be included in the grid, and (2) a balance between convergence and cost, so we choose the cutoff energy to be 40 Hartree, and the Brillouin-zone sampling mesh parameters for the k-point set are 4×4×4.

2.2 GW approximation

Although, a number of schemes considering many-body effects have been forwarded, one of the very successful schemes for the evaluation of the self-energy is the GW approximation given by Hedin and developed as a practical computational approach for real materials by Hybertsen and Louie[38]. The GW approximation for the electron self-energy is the state-of-the-art method for predictive calculations of the band gap and of other excited state properties. It yields excellent results for semiconductors and insulators[19, 25, 26].

In the GW approximation, the wave function and eigenvalue of a quasiparticle in a crystal are obtained by solving the Dyson equation[38]

$$[T+V_{ext}+V_H]\Psi_{nk}(\vec{r})+\int d\vec{r}\,\Sigma(\vec{r},\vec{r}\,';E_{nk}^{qp})\Psi_{nk}(\vec{r})'=E_{nk}^{qp}\Psi_{nk}(\vec{r}) \quad (1)$$

where T is the kinetic energy operator; V_{ext} is the external potential due to the ions; V_H denotes the Hartree potential arising from the Coulomb interaction between electrons; Ψ_{nk} is the wavefunction; Σ is the non-local energy dependent non-Hermitian self-energy operator which includes the many-body effects of exchange and correlation between electrons. As Σ is non-Hermitian, the eigenvalue E_{nk}^{qp} is complex and its imaginary part gives the lifetime of the quasiparticle. n and k are the band and K-piont indices, respectively. Hedin[24] expanded the self-energy operator in a perturbation series in terms of fully screened Coulomb interaction. If one retains only the first term in the expansion, one obtain the so-called GW approximation[19]. In GW approximation, Σ is expressed as[38]

$$\Sigma(r,r';E)\cong\frac{i}{2\pi}\int d\omega e^{-i\omega 0^{+}}G(r,r';E-\omega)W(r,r';\omega) \quad (2)$$

where G is Green's function and W is the screened Coulomb interaction. The dynamical screened Coulomb interaction W is given by $W=\varepsilon^{-1}V_c$ (V_c is the bare Coulomb interaction and ε is the dynamical dielectric function, and matrix elements of the inverse dielectric matrix between the reciprocal lattice vectors $(\vec{G},\vec{G}')$ are expressed as $\varepsilon^{-1}_{\vec{G},\vec{G}'}(\omega)$.

For the calculation of the Green's function, there are usually two approximations: one is the assumption of infinite lifetime for the quasiparticle, and the second is the choice of GGA eigenfunctions as the quasiparticle wave functions while the finite lifetime of the quasiparticle is neglected in this approach. To the screened Coulomb interaction, a generalized form of the Levine-Louie model dielectric matrix extended to finite frequencies using a generalized plasmon-pole model. This model dielectric function is known to give reliable results for various semiconductors and requires only the dielectric constant ε_∞ as an input[25]. The quasiparticle energy E_{nk}^{qp} is expressed as the GGA energy eigenvalue plus a many body correction as

$$E_{nk}^{qp}=\varepsilon_{nk}^{GGA}+\langle n\vec{k}|\Sigma(E_{nk}^{qp})-V_{xc}^{GGA}|n\vec{k}\rangle \quad (3)$$

with ε_{nk}^{GGA} and $\langle n,k|$ as the eigenvalue and eigenfunction at k for band n in GGA. V_{xc}^{GGA} is the GGA exchange-correlation potential; $\Sigma(E_{nk}^{qp})$ is the self-energy for the quasiparticle energy E_{nk}^{qp}.

For GW approximation, we firstly calculate for converged ground state to get Kohn-Sham data, then compute the independent-particle susceptibility matrix and the dielectric matrix on the basis of these available Kohn-Sham data and compute the self-energy matrix element at the given k-point to derive the GW eigenvalues for the target states at this k-point.

3 Results and discussion

3.1 Structural properties

Firstly, the structural properties of the binary compounds CaX (X=S, Se, Te) in NaCl structure are analyzed. In order to calculate the ground state properties of CaX (X=S, Se, Te), the total energies are calculated using DFT-LDA for different volumes. The plots of calculated total energies versus different values of volume for these compounds are given in Figs. 1～3. By fitting a second degree polynomial from the E-V curves, we obtain the equilibrium primitive cell volume V_0 (corresponding to the equilibrium lattice constant a_0). The optimized equilibrium lattice constants of the CaX (X=S, Se, Te) are listed in Tab. 1, which also contains results of the available theoretical[3, 4, 8, 13] and experimental values[1] in literatures. Our results are in good agreement with experimental results. And we also found that for all compounds the GGA always overestimates the lattice parameter while the LDA underestimates it. These findings are consistent with the general trend of these approximations. Although, the equilibrium lattice constants determined from our calculations by using LDA are slightly less than the experimental data and precent errors are with 1%～1.5%. We believe that our results are reasonable and accurate. The lattice constants of a solid increase in the order, CaS, CaSe and CaTe, because of an increase in the size of the anion.

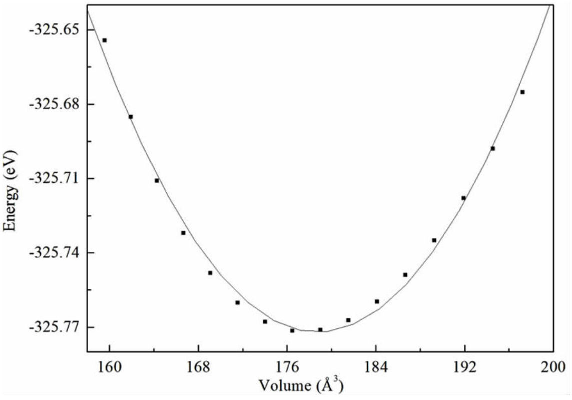

图 1 CaS 的能量一体积曲线

Fig. 1 Total energy as function of volume for CaS

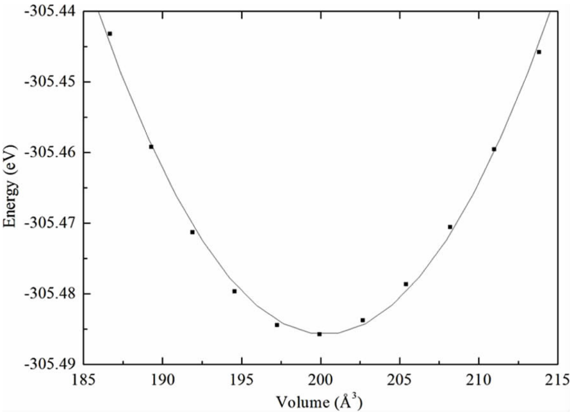

图 2 CaSe 的能量一体积曲线

Fig. 2 Total energy as function of volume for CaSe

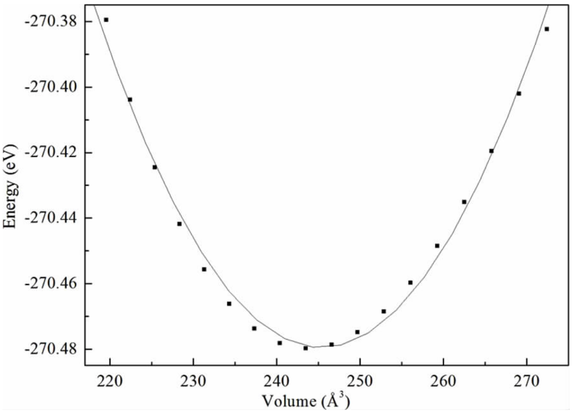

图 3 CaTe 的能量一体积曲线

Fig. 3 Total energy as function of volume for CaTe

表 1 CaX (X=S, Se, Te) 的晶格常数(Å)与其它理论值及实验值的比较

Tab. 1 Lattice constants (Å) of CaX (X=S, Se, Te) and their comparison with other theoretical and experimental data

Materials	Present a(Å)	Expt. [1]	Other theoretical works	
			LDA	GGA
CaS	5.63	5.689	5.57[3]	5.72[3]
			5.564[8]	5.717[8]
			5.610[13]	5.701[4]
CaSe	5.85	5.916	5.790[8]	5.968[8]
			5.84[13]	
CaTe	6.25	6.348	6.208[8]	6.396[8]
			6.25[13]	

3.2 Electronic properties

The electronic band structures of CaX (X=S, Se, Te) have been calculated at the theoretical equilibrium lattice constant, rather than at the experimental one. This choice appears to be more consistent with the structural calculations, and comparison with experimental data yields better results both qualitatively and quantitatively. The electronic band structures of CaX (X = S, Se, Te) with LDA functional are shown in Figs. 4～6. Figs. 4～6 show that CaX (X = S, Se, Te) have an indirect gaps with the maximums of the valence band at Γ and that the minimums of the conduction band at X, agreeing with previous DFT-LDA calculation except the results (Γ－Γ) given by Pandey *et al*. using the Hartree Fock method[15]. Most of the compounds examined till date by experimental methods have indirect gaps produced by Γ－X transitions in the NaCl structure[26, 39]. So we have reason to believe that these compounds are indirect band gap semiconductors. The minimum gap values are 2.18 eV for CaS, 1.88 eV for CaSe and 1.33 eV for CaTe by using LDA calculation in Figs. 4～6 respectively. It can be seen that the calculated energy gap values decrease with the increase of the size of the chalcogen atom. This finding is consistent with the general trend of chalcogenide compounds[25, 26]. All of band gap values calculated are shown in Tab. 2 and compared with other theoretical works and available experimental data. Our results with LDA calculations are in good agreement with the earlier theoretical calculations except the results with HF method. But these results are much lower than the experiment values about 38% ～ 52%[1, 2]. These results are expected since the LDA always underestimates the band gap of semiconductors. This is mainly due to the fact that they have simple forms that are not sufficiently flexible for accurately reproducing both exchange-correlation energy and its charge derivative[8]. Similar trend has been observed in other theoretical papers which apply LDA to the band structures of semiconductors and insulators[40, 41].

To get a reliable band gap value, we use the GW approximation to correct the band gap. We only considered three high symmetry points of the Brillouin zone for CaX (X=S, Se, Te) from the point of the computer resources, which are Γ, X and L, respectively. The direct and indirect band gap values in GW approximation and other theoretical and experimental values are summarized in Tab. 2. The GW approximation does not significantly change the top of valence band and the bottom of conduction given by the LDA calculation. The top of valance band is also at Γ point, and the bottom of conduction band is at X point for CaX (X=S, Se, Te). They are also indirect band gap semiconductors. However, compared to the results of the LDA calculations, the band gaps are significantly enlarged by the GW approximation. The calculated minimum band gaps in GW approximation are 3.903 eV for CaS, 3.22 eV for CaSe and 2.34 eV for CaTe, respectively. For the minimum band gap of CaS, our GW approximation result is lower than the experimental data of 4.434[5] and 4.52 eV[14], but higher than the experimental datum of of 3.5 eV[12]. For the CaSe, our result by GW approximation is most close to the experimental data. Our calculations in GW approximation are more close to the experimental data than other theoretical values, despite the results are smaller. For the CaTe, the GW band gap is larger than the LDA band gap by 1.01 eV. This corresponds to approximately 76% of the LDA band gap energy. It may serve as prediction calculation because of the lack of experimental value. But our results of the CaS and CaSe in GW approximation are in good agreement with experimental data. And, the GW approximation has been successfully tested in semiconductors and insulators. Hence, we believe that the band gap value of CaTe by GW approximation is very reliable and can be used as good reference for other studies.

The LDA is the ground state theory, i. e. the solution based on the Kohn-Sham equation is a powerful tool for studying the ground state properties in many particle systems, but it is not good to describe the excited state properties. Because the first principles computation of excited states is more complexity than ground-state calculations. The key problem is that the exchange-correlation interaction in excited states is different from the ground states. Compared with the LDA, self-energy substitutes the exchange correlation potential in the GW approximation. Namely, we use the Σ in the quasiparticle equation (1) instead of the V_{xc}^{LDA} in the Kohn-Sham equation. So, the GW commonly obtains a lower energy for the valence band and higher energy for the conduction band. As a consequence, the band gap is larger than that of LDA and GGA.

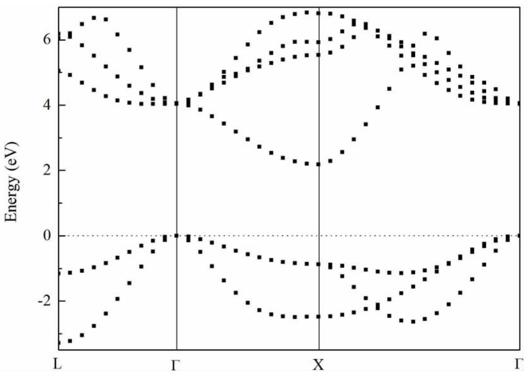

图 4　CaS 的 LDA 能带结构图

Fig. 4　Band structure in LDA for CaS

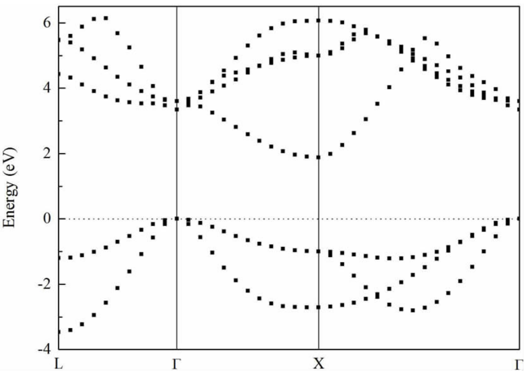

图 5　CaSe 的 LDA 能带结构图

Fig. 5　Band structure in LDA for CaSe

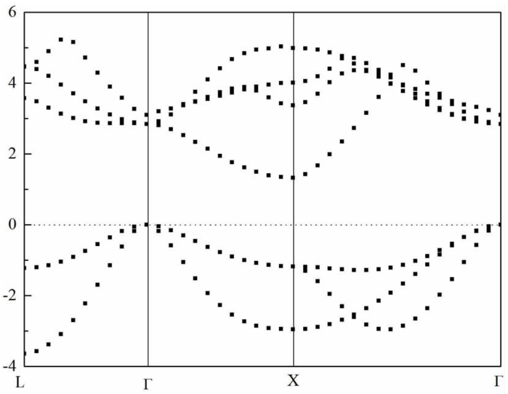

图 6　CaTe 的 LDA 能带结构图

Fig. 6　Band structure in LDA for CaTe

表 2　Ca*X* (*X*=S, Se, Te)布里渊区高对称点的带隙值(eV)

Tab. 2 The band gap values (in eV) of Ca*X* (*X*=S, Se, Te) at high symmetry points of Brillouin zone

structure	reference	Γ−Γ	X−X	Γ−X
CaS	This work GW	5.88	4.88	3.903
	This work LDA	4.04	3.06	2.18
	Expt. values	5.80[5]	5.343[5]	4.434[5]
			5.33[14]	4.52[14]
				3.5[12]
	Other calculations	4.25[3]	3.04[3]	2.15[3]
		3.9[3]	2.85[3]	1.9[3]
		4.453[13]	3.123[13]	2.39[8]
		7.6[15]	12.64[15]	3.18[8]
				2.36[13]
				10.39[15]
CaSe	This work GW	4.669	4.355	3.22
	This work LDA	3.35	2.88	1.88
	Expt. values		4.898[5]	3.85[5]
			4.92[14]	3.93[14]
	Other calculations	3.539[15]	2.889[15]	2.10[8]
				2.81[8]
				1.98[15]
CaTe	This work GW	3.951	3.647	2.34
	This work LDA	2.85	2.51	1.33
	Other calculations	3.086[15]	2.467[15]	1.57[8]
				2.23[8]
				1.35[15]

4　Conclusions

In this work, we have made an investigation of the structures and electronic properties of Ca*X* (*X*=S, Se, Te) in NaCl structure. The calculated lattice parameters of Ca*X* (*X*=S, Se, Te) using LDA are consistent with the experimental values. We have calculated the band structures of the Ca*X* (*X*=S, Se, Te) by the LDA method and corrected the band gaps by the GW methods. Because the GW approximation considers the many body effects, and the substitution of self-energy in GW approximation for the exchange correlation potential in LDA, the band gaps are remarkably increased from 2.18 to 3.903 eV for CaS, 1.88 to 3.22 eV for CaSe and 1.33 to 2.34 eV for CaTe, respectively. And the GW approximation does not change the top of valence band and the bottom of conduction given by the LDA calculation. The calculated band gaps along the Γ−X direction for CaS and CaSe by using the GW approximation agree well with the experimental data. Though there is no experimental data for CaTe, we believe that our calculated band gap of CaTe in GW approximation is very reliable.

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