Density-functional theory investigation of energy gaps and optical properties of $Hg_{1-x}Cd_xTe$ and $In_{1-x}Ga_xAs$*

Guo San-Dong(郭三栋)† and Liu Bang-Gui(刘邦贵)

Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, *China*

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We use a modified Becke–Johnson exchange plus a local density approximation correlation potential within the density functional theory to investigate the electronic structures of $Hg_{1-x}Cd_xTe$ and $In_{1-x}Ga_xAs$ with x being 0, 0.25, 0.5, 0.75, and 1. For both of the two series, our calculated energy gaps and dielectric functions (real part ε_1 and imaginary part ε_2) are in agreement with the corresponding experimental results with x being between 0 and 1. The calculated zero-frequency refractive index varies greatly with x for $Hg_{1-x}Cd_xTe$, but changes little with x for $In_{1-x}Ga_xAs$, which is consistent with the real parts of their dielectric functions. Therefore, this new approach is satisfactory to describe the electronic structures and the optical properties of the semiconductors.

Keywords: semiconductor, gap, optical property

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1. Introduction

$Hg_{1-x}Cd_xTe$ alloys can have different band gaps through changing x, and thus can provide an unprecedented degree of freedom in infrared (IR) detector design. They may become the most important material for detector applications in the entire IR range.[1] Related HgTe/CdTe quantum-well structures are predicted theoretically to be two-dimensional quantum spin hall topological insulators, which has been confirmed by experiments.[2–4] The semiconductor $In_{1-x}Ga_xAs$ is an important model material for high speed devices, such as high electron mobility transistors and field-effect transistors, due to its small effective electron mass and high electron mobility. It can be used to fabricate quantum confinement heterostructure lasers. High-performance optical properties can be obtained by controlling the indium composition and the thickness of the layers in the quantum wells.[5,6] It is highly desirable to elucidate the x-dependent electronic structures and optical properties of these two series of semiconductors for further applications.

Since the energy gap is underestimated by the local density approximation (LDA) and the generalized gradient approximation (GGA), some further approximations are usually needed to make the first-principles electronic gaps and optical properties comparable with the experimental results. Fortunately, a modified Becke–Johnson exchange plus local density approximation correlation potential (mBJLDA) was proposed recently by Tran and Blaha,[7] which can be used to produce accurate semiconductor gaps. So far, several groups have used the mBJLDA potential for the calculation of the electronic properties of different families of solids, confirming that mBJLDA band gaps are improved for a wide range of different materials.[8–13] In this paper, we use the mBJLDA approach within the density functional theory (DFT) to investigate the electronic structures and the optical dielectric functions of $Hg_{1-x}Cd_xTe$ and $In_{1-x}Ga_xAs$ with x being 0, 0.25, 0.5, 0.75, and 1. Our results show that the calculated energy gaps and the optical properties agree with related experimental results of $Hg_{1-x}Cd_xTe$ and $In_{1-x}Ga_xAs$ with x being in the range of from 0 to 1. More detailed results will be presented in the following.

We will give the computational details in the next section. Our main results will be presented in the third

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†Corresponding author. E-mail: gsd@iphy.ac.cn

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section. In the fourth section, we will discuss our results and give our conclusion.

2. Computational details

We use the full-potential linearized augmented-plane-waves method within the density functional theory,[14,15] which is implemented in the package WIEN2k.[16] We use the mBJLDA for the exchange–correlation potential[17,7] to perform our main DFT calculations, and take the popular GGA by Perdew, Burke, and Ernzerhof (GGA-PBE)[18] to optimize the volume and the internal position parameters. The full relativistic effects are calculated with the Dirac equations for the core states, and the scalar relativistic approximation is used for the valence states.[19−21] The spin–orbit coupling is neglected, because it has little effect on our results. We use 2000 k-points in the first Brillouin zone for the self-consistent calculation and 20000 k-points for the optical property calculation. We make the harmonic expansion up to $l_{\max} = 10$ in each of the atomic spheres and set $R_{\rm mt} \times k_{\max} = 8$. The radii of the atomic spheres of Hg, Cd, Te, In, Ga, and As are set to $2.5a_0$, $2.5a_0$, $2.5a_0$, $2.33a_0$, $2.33a_0$, and $2.33a_0$, respectively, where a_0 is the Bohr radius. The volumes are optimized in terms of the total energy and the internal position parameters with a force standard of 2 mRy/a.u. The self-consistent calculations are considered to be converged when the integration of the absolute charge-density difference between the input and the output electron densities is less than $0.0001|e|$ per formula unit, where e is the electron charge.

3. Main calculated results

At first, we construct the smallest unit cell by substituting Cd (Ga) for Hg (In) in the zincblende structure of $Hg_{1-x}Cd_xTe$ ($In_{1-x}Ga_xAs$) with x equaling 0, 0.25, 0.5, 0.75, and 1, and then optimize their volumes and internal position parameters by using the popular GGA. The optimized lattice constants are summarized in Table 1. For $Hg_{1-x}Cd_xTe$, the lattice constants vary very little with x, increasing by 0.45% from CdTe to HgTe. The lattice constants for $Hg_{1-x}Cd_xTe$ are larger than those obtaind by the LDA in Ref. [22], because for semiconductors, the lattice constants obtained by the GGA usually are a little larger than the experimental values, while those obtained by the LDA are a little smaller than the experimental values. For $In_{1-x}Ga_xAs$, the lattice constants gradually change with x, increasing by 7.6% from GaAs to InAs. As is well know, the GGA and the LDA underestimate the gaps of semiconductors. Therefore, we use an improved exchange–correlation method including the modified Becke–Johnson exchange potential to calculate the electronic structures of $Hg_{1-x}Cd_xTe$ and $In_{1-x}Ga_xAs$. This new method improves semiconductor gaps and d-state positions for numerous materials. We summarize the gap data in Table 1 for $Hg_{1-x}Cd_xTe$ and $In_{1-x}Ga_xAs$, and compare the gaps calculated with the mBJLDA with the experimental ones for $Hg_{1-x}Cd_xTe$[23] and $In_{1-x}Ga_xAs$[24] in Fig. 1. The gap of HgTe is -0.03 eV, the negative sign means that the Fermi energy crosses the conduction band. The gap increases from –0.03 eV to 1.57 eV for $Hg_{1-x}Cd_xTe$ and from 0.31 eV to 1.23 eV for $In_{1-x}Ga_xAs$ with x varying from 0 to 1. The gap value 1.23 eV in the case of GaAs is obtained because we use the optimized lattice constant 5.752 Å. The larger value given in Ref. [7] can be obtained if we use the experimental lattice constant. From Fig. 1, we can see that for $Hg_{1-x}Cd_xTe$, the gaps agree well with the experimental values, and for $In_{1-x}Ga_xAs$, the gaps calculated with the mBJLDA are lower than the experimental values for larger x.

Table 1. Lattice constants a optimized with the GGA, and gaps and the zero-frequency refractive index $n(0)$ of $Hg_{1-x}Cd_xTe$ and $In_{1-x}Ga_xAs$ calculated with the mBJLDA.

	$Hg_{1-x}Cd_xTe$			$In_{1-x}Ga_xAs$		
x	a /Å	Gap/eV	$n(0)$	a /Å	Gap/eV	$n(0)$
0	6.660	-0.03	3.70	6.192	0.31	3.38
0.25	6.654	0.22	3.30	6.076	0.46	3.35
0.5	6.647	0.62	3.00	5.975	0.58	3.29
0.75	6.639	1.05	2.74	5.867	0.85	3.26
1	6.630	1.57	2.55	5.752	1.23	3.19

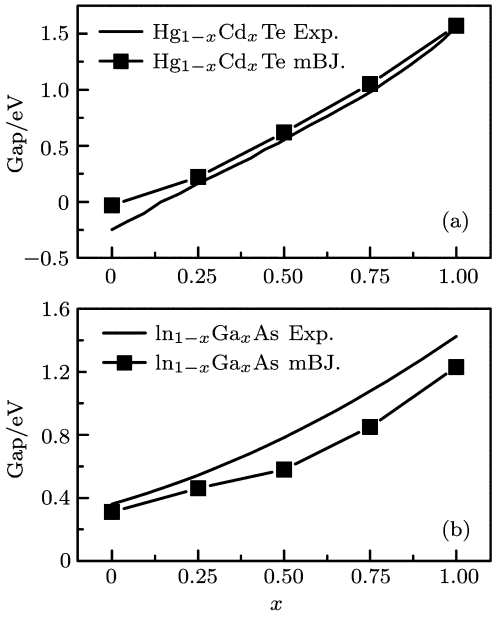


Fig. 1. Energy gaps of $Hg_{1-x}Cd_xTe$[23] (a) and $In_{1-x}Ga_xAs$[24] (b) with different x calculated with the mBJLDA compared with those measured experimentally.

We present the energy bands with the Hg character calculated with the mBJLDA for $Hg_{1-x}Cd_xTe$ and those with the In character calculated for $In_{1-x}Ga_xAs$ in Fig. 2. As x changes from 0 to 1, the space group of the crystal structure undergoes a change of 216, 215, 115, 215, and 216, and the atom number in the unit cell changes from 2 to 8, 4, 8, 2, which can be seen from the number of energy bands. There is a band cross point near the Fermi energy at high symmetry Γ point for HgTe in both bands calculated with the mBJLDA and the GGA. However, the InAs has a direct energy gap of 0.31 eV according to the calculation with the mBJLDA, while the conduction bands calculated with the GGA are crossed by the Fermi level. For both $Hg_{1-x}Cd_xTe$ and $In_{1-x}Ga_xAs$, the gap is a direct band one at the Γ point, and we use the same Brillouin zone as that of the face-centred cubic structure for convenience in comparing energy bands of different x (note: The path is not always the lines connecting the high symmetry points).

The real part ε_1 and the imaginary part ε_2 of the dielectric functions calculated with the mBJLDA are presented in Fig. 3 for $Hg_{1-x}Cd_xTe$[25] and in Fig. 4 for $In_{1-x}Ga_xAs$,[26] and related room-temperature experimental results are also shown for comparison. The calculated dielectric functions as functions of photon energy are consistent with the experimental results for both $Hg_{1-x}Cd_xTe$ and $In_{1-x}Ga_xAs$. For different x, the main differences of the dielectric functions are between 0 eV and 6 eV for $Hg_{1-x}Cd_xTe$. The real part ε_1 and the imaginary part ε_2 between 0 eV and 2 eV increase with x changing from 1 to 0, and the x dependence becomes small at the higher photon energy, which are consistent with the experimental results. For $In_{1-x}Ga_xAs$, the x dependence of the dielectric functions, both the real part ε_1 and the imaginary part ε_2, is smaller than that for $Hg_{1-x}Cd_xTe$. We also calculate the zero frequency refractive indexes $n(0)$ for

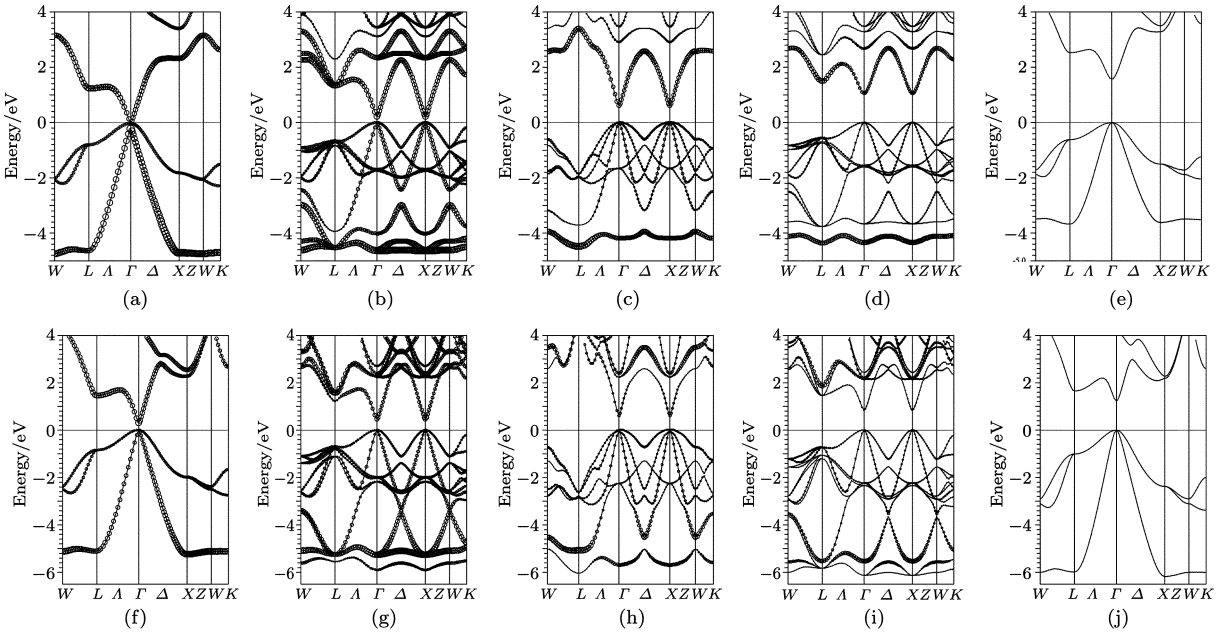


Fig. 2. Energy bands of $Hg_{1-x}Cd_xTe$ ((a)–(e)) and $In_{1-x}Ga_xAs$ ((f)–(j)) calculated with the mBJLDA with x equaling to 0, 0.25, 0.5, 0.75, and 1 (from left to right). The diameter of a dot in a band is proportional to either Hg or In weight at that point. The Fermi energy E_F is set to be 0.

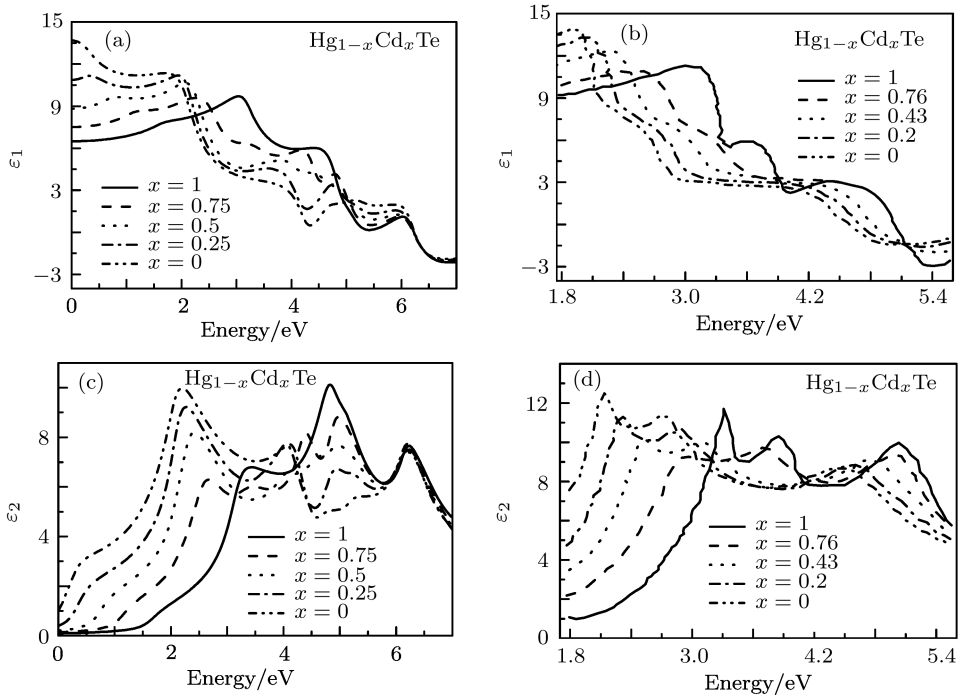


Fig. 3. Real parts ε_1 and imaginary parts ε_2 of dielectric functions of $Hg_{1-x}Cd_xTe$ (with $x = 0$, 0.25, 0.5, 0.75, 1) calculated with the mBJLDA ((a) and (c)) and some room-temperature experimental results ((b) and (d)).[25]

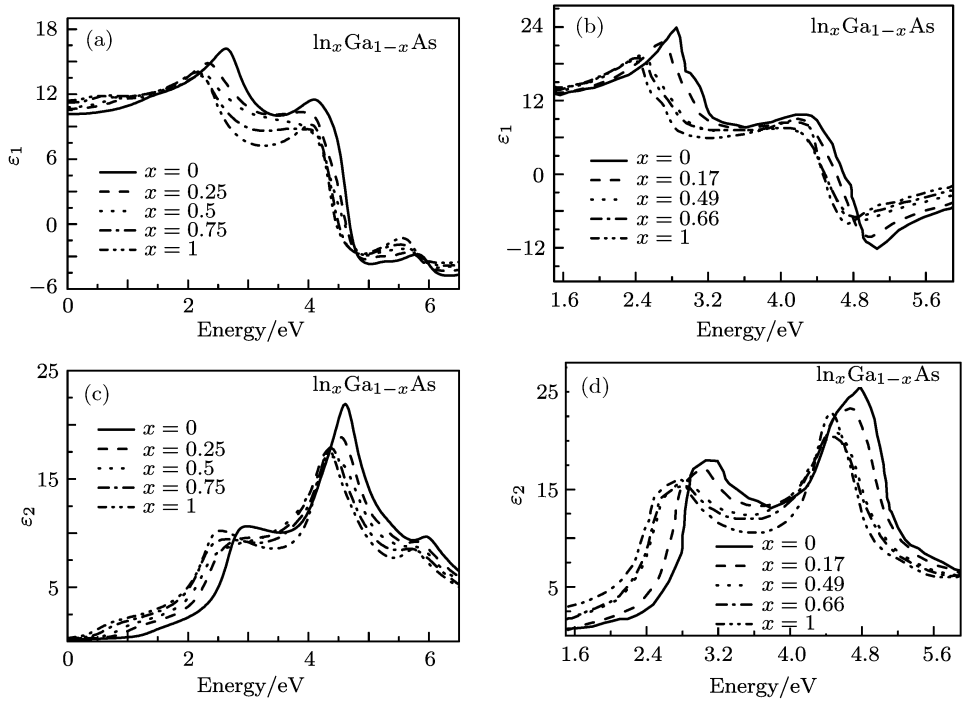


Fig. 4. Real parts ε_1 and imaginary parts ε_2 of dielectric functions of $In_{1-x}Ga_xAs$ (with $x = 0$, 0.25, 0.5, 0.75, 1) calculated with the mBJLDA ((a) and (c)) and some room-temperature experimental results ((b) and (d)).[26]

$Hg_{1-x}Cd_xTe$ and $In_{1-x}Ga_xAs$. The related data are summarized in Table 1. The calculated $n(0)$ decreases with x for both cases. The x dependence of the calculated $n(0)$ for $Hg_{1-x}Cd_xTe$ is substantially larger than that for $In_{1-x}Ga_xAs$. This is accordance with the real parts of the dielectric functions.

4. Discussion and conclusion

Semiconductor gaps are important parameters for device design, however the DFT calculation with the LDA or the GGA usually underestimates the gaps. $Hg_{1-x}Cd_xTe$ (x = 0.250, 0.375, 0.500, 0.625, 0.875, 1.000) has been studied by using first-principles calcu-

lations with the LDA,[22] the LDA-calculated gaps are substantially smaller than the experimental values. It has been proved that the mBJLDA potential improves semiconductor gaps for numerous semiconducotrs.[7] For HgTe, both the mBJLDA and the GGA calculations produce no gap, which is consistent with experiments. For InAs, the GGA calculations produce no gap, while the mBJLDA gives a correct gap comparable with the experimental value. Therefore, the mBJLDA does not merely enlarge the gap, but can produce accurately the gap in some cases where other exchange–correlation potentials cannot yield the nonzero gap. The optical properties can reflect the outline of the energy structure, not just the gap. The mBJLDA yields the optical properties, which are in agreement with the room temperature experiment for both $Hg_{1-x}Cd_xTe$ and $In_{1-x}Ga_xAs$. The substantial improvement shows that the mBJLDA gives a better description to the kinetic effects of electrons than either the LDA or the GGA.

In summary, we have used a state-of-the-art DFT method with the mBJLDA potential to investigate the electronic structures of $Hg_{1-x}Cd_xTe$ and $In_{1-x}Ga_xAs$ with x being 0, 0.25, 0.5, 0.75, and 1. For both $Hg_{1-x}Cd_xTe$ and $In_{1-x}Ga_xAs$, our calculated energy gaps are in accordance with the related experimental results for x being between 0 and 1. We also calculate the real part ε_1 and the imaginary part ε_2 of the dielectric functions of $Hg_{1-x}Cd_xTe$ and $In_{1-x}Ga_xAs$, showing that the calculated results are consistent with the experimental ones. Our x dependence of the dielectric functions agrees well with the experiment. We also calculate the zero-frequency refractive index $n(0)$ with the mBJLDA. Our study shows that the calculated $n(0)$ decreases with the increasing x, and the x dependence of $Hg_{1-x}Cd_xTe$ is substantially larger than that of $In_{1-x}Ga_xAs$, which is consistent with the corresponding real parts of the dielectric functions. Therefore, the mBJLDA is satisfactory to describe the electronic structures and the optical properties of the semiconductors.

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