Pristine and doped chromium arsenide (CrAs) in six different crystal structures is systematically studied to investigate the structural, magnetic, and optical properties for real applications by first-principles calculations. First, it is found that the ground-state structure is an orthorhombic MnP-type structure with antiferromagnetic spin order. The rocksalt structure is a low-energy metastable phase and a ferromagnetic metal with high spin polarization at the Fermi level. Second, the NiAs structure and MnP structure have a higher absorption coefficient than other structures in the infrared region and ultraviolet region, respectively. In the visible region, the wurtzite and zincblende structures are more transparent than other structures. At last, the substitution of Cr by Ti and the substitution of As by Te can lead to a phase transition in ground-state structure and ground-state magnetic order, respectively. These results can promote the application of the CrAs system into spintronics and optoelectronics.

1. Introduction

Spintronics (or magnetoelectronics),[1] which adds the spin degree of freedom to conventional electronic devices, has several advantages like increasing data processing, decreased electric power consumption, and nonvolatility.[2–4] In 1983, de Groot et al. predicted half Heusler alloys NiMnSb and PtMnSb[5] to be half-metallic (HM) materials, which have 100% spin polarization at the Fermi level. Transition metal pnictides (e.g., CrAs and VAs) have various phases including zincblende (ZB), wurtzite (WZ), hexagonal NiAs (NA), and orthogonal MnP (MP)-type structures.[6] These materials have rich magnetic orders and compatibility with the traditional group III-V or II-VI semiconductors (e.g., GaAs, ZnTe).[6] Thus, it is significant to explore the electric and magnetic properties of transition metal pnictides.[7]

Chromium arsenide (CrAs) exhibit an MP-type orthorhombic structure at low temperature.[8,9] T. Ito et al. predicted that MP-type CrAs shows a double-spiral antiferromagnetic (AFM) magnetic order with a magnetic moment of 1.7 μB per Cr atom.[10] Kotegawa et al. observed a first-order antiferromagnetic-paramagnetic transition at 265 K, which is interpreted as an electronic transition between localized and collective states.[11] Svitlana Polesya et al. proved that nearest-neighbor and next nearest-neighbor Cr–Cr interactions in CrAs are ferromagnetic (FM) and AFM, respectively.[12] They predicted that the magnetic phase transition temperature from the paramagnetic to the double-helical magnetic structure is about 270 K, consistent with the experiment value.[13] Wu et al.[14] and Kotegawa et al.[15] independently discovered pressure-induced unconventional superconductivity in the vicinity of AFM order in MP-type crystal structure CrAs. Carmine et al. predicted that CrAs may be a weakly correlated material with the Fermi surface exhibiting a 2D behavior, which suggests a close link between the appearance of the superconductivity and the external pressure.[16] Moreover, W. Wu et al. observed that MP-type CrAs show a Fermi-liquid behavior with a T²-dependent resistivity at low temperature.[17]

Much research effort has also been devoted to other metastable phases of CrAs. N. Kazama et al.[18] observed that CrAs occurs as a structural phase transition from the MnP structure to NiAs structure at high T = 769 K. Another meta-stable ZB-type CrAs has been fabricated on GaAs(001) substrates by molecular-beam-epitaxy (MBE).[19,20] The experiment and theory confirmed that ZB-type CrAs have well-pronounced HM behavior with high Curie temperature above 400 K.[20,21] A. Azouaoui et al. have shown that ZB-CrAs is more stable in the ground state with a FM configuration.[22] Under 5 GPa pressure, CrAs experienced structural and magnetic transition from FM ZB-CrAs structure to AFM Pnma structure.[23] Xie et al.[24] predicted WZ-type CrAs to be HM ferromagnet. Besides, the magnetic properties of CrAs are very sensitive to substitutions of other elements. Suzuki and Ido reported that the substitution of only 7.5% of phosphorus for...
arsenic in CrAs yields a collapse of the double-spiral magnetic order.\[24\] Meanwhile, the transition temperature of CrAs is very sensitively influenced by other 3d metal substitutions for the Cr.\[25,26\] The previous theoretical research paid little attention to the doping effect on the structural properties as well as the optical properties of CrAs system. It is meaningful to explore the structural, magnetic, optical, and electronic structural properties of pristine and doped CrAs in various structures.

Here, we focused on a systematical study of CrAs in various crystal structures utilizing the density functional theory. We performed first-principles calculations based on CrAs in six phases including the rocksalt (RS), cesium-chloride (CC), ZB, WZ, NA, and MP phase. Then we displayed their optical properties. At last, we report the doping effect on the structural and magnetic properties of CrAs. The computational details are given in the next section. The main results and discussion will be presented in the third section. We shall give our conclusion in the fourth section.

2. Methodology

Our density functional theory (DFT) calculations were performed by using the Vienna ab-initio simulation package (VASP).\[27–29\] This code solves the Kohn–Sham equations within the pseudo-potential approximation.\[10] The generalized gradient approximation (GGA) to the exchange-correlation potential in form of the Perdew, Burke, and Ernzerhof (PBE)\[31\] functional was used in this work. After convergence tests, an energy cutoff of 650 eV for the plane-wave expansion was selected. The K-points, sampling over the irreducible Brillouin zone, were generated by Monkhorst–Pack scheme.\[32\] We used K-points mesh of 9 × 9 × 9 for RS, CC, ZB; 11 × 11 × 7 for WZ, NA; and 7 × 11 × 7 for MP type, respectively. The convergence of the results concerning k-point sampling has been carefully checked. To explore the magnetic properties of CrAs, we have calculated the total energy of nonmagnetic (NM), FM, and different AFM phases for six crystal structures. All the structures have been optimized to achieve the minimum energy by accurate relaxation of the atomic positions up to the energy accuracy of 10−5 eV. The optical properties of solids are described by dielectric functions.\[33,34\]

The cohesive energy of CrAs compounds was calculated by following formula\[35\]

\[
E_c = \frac{1}{2} \left( E_{tot}^{CrAs} - E_{atom}^{Cr} - E_{atom}^{As} \right)
\]

(1)

where \( E_{tot}^{CrAs} \) is the total energy per formula unit of CrAs compound, \( E_{atom}^{Cr} \) and \( E_{atom}^{As} \) are the energy of isolated Cr and As atoms, respectively.

3. Results and Discussion

3.1. The Structural Analysis of Six Structures

1) RS-type CrAs has a space group of \( Fm\overline{3}m \) (No.225). It composes of two face-centered cubic lattices, shifted by the vector (0.5, 0.5, 0.5), which results in octahedral coordination for both cations and anions; 2) CC-type CrAs has a space group of \( Pm\overline{3}m \) (No.221). The CC structure can be described as two interpenetrating simple cubic lattices shifted by the vector (0.5, 0.5, 0.5) along the body diagonal of the conventional cube. Each anion in a given sublattice has 8 nearest neighboring cations on the other sublattice, there are 6 second nearest neighbors of the same type sublattice; 3) ZB-type CrAs has a space group \( F\overline{4}3m \) (No.216). The ZB structure is similar to that of a diamond with two interpenetrating face-centered cubic lattices displaced by the vector (0.25,0.25,0.25) along the body diagonal of the conventional cube. The coordination number is 4 for each atom; 4) WZ-type CrAs has a space group \( P6_3mc \) (No.186). The WZ structure is regarded as a distorted ZB-type structure with small shifts of atomic positions. There are four atoms of two different types in the unit cell (see Figure 1d). Each atom is surrounded by a tetrahedron of atoms of opposite sort hexagonal analog to the ZB structure and has the same local environment if one assumes the ideal c/a ratio and internal parameters u of 3/8 for the anion site; 5) NA-type CrAs has a space group \( P6_3/mmc \) (No.194), as shown in Figure 1e. It has four atoms in the primitive unit cell. As atoms form a lattice like the hexagonal close-packed structure, and Cr atoms a simple hexagonal lattice. As distortion and shifts are small, the NA and MP structures are similar. However, even the slight difference affects magnetic properties through the change of electronic structure; and 6) MP-type CrAs has a space group \( Pna \) (No.62). The orthorhombic MnP-type structure is regarded as a distorted NiAs-type structure with small shifts of atomic positions.\[36\] The structure, illustrated in Figure 1f, shows that each Cr atom is coordinated with six As atoms in irregular octahedral coordination. Each As atom is surrounded by six Cr atoms, arranged at the corners of a distorted trigonal prism. This structure possesses a space-inversion symmetry.

3.2. The Ground-State and Metastable Structures

In the fully optimized calculations, all lattice parameters and internal atomic positions were relaxed to find out the ground state of CrAs. By fitting the Birch–Murnaghan equation of state to the obtained total energies as a function of volume, the structural properties of the systems were determined.

We first investigated the NM, FM, and AFM states of CrAs in the MP-type structure. As seen in Figure 2b, the MP-type CrAs in AFM state is energetically more stable compared to the FM and NM state over a wide range of lattice volumes. This is consistent with the experimental observation that MP-type CrAs is in the AFM state.\[37\] The equilibrium lattice volume of AFM MP-type CrAs is found to be 31.28 Å³.

Then the calculated total energies versus formula volume for CrAs in six crystal structures are displayed in Figure 2a. For the MP and NA structures only AFM phases are presented because the NM and FM phases are always higher in total energy (see Figure 2b). For the other four structures: RS, CC ZB, and WZ, we choose ZB as a representative. The calculated total energies as a function of crystal volume for NM, FM, and AFM states of CrAs in ZB-type structure are plotted in Figure 2c. As seen in this figure, the total calculation indicates that the FM state is the most stable for this structure. This is consistent with the previous
work that ZB-type CrAs is an FM state\textsuperscript{[38,19]} Thus, only the FM phases of ZB, CC, WZ, RS are presented in Figure 2a because the NM and AFM phases are always higher in total energy. The results of structural properties and magnetic moments of six structures for CrAs together with theoretical and experimental results are summarized in Table 1.

As seen in Table 1, the cohesive energy $E_c$ of CrAs phases is negative. The smaller the value of $E_c$, the more stable the structure is. Fully optimized MP-type CrAs in the AFM state is lower in energy than any other phase, so it is the ground-state phase, which agrees well with the experimental ground state, and theoretical structural parameters in this state are also in agreement with experimental values.\textsuperscript{[8]} The NA-type CrAs in the AFM state is 40 meV higher than MP-type CrAs in the AFM state (see Figure 2a). However, the MP-type CrAs in the FM state has a higher energy of 36 meV than MP-type CrAs in the AFM state (see Figure 2b). Thus, the energy of MP-type CrAs in the FM state is slightly smaller than the NA-type CrAs in AFM state and is the second-most stable phase. This may explain that the new metastable FM orthorhombic structure CrAs epilayers can be grown on GaAs(001) in a recent experiment,\textsuperscript{[42]} and it also agrees with Hashemifar’s results.\textsuperscript{[37]}

The metastable structure with the energy next to that of the MP and NA structure is the CC structure (see Figure 2a) which prefers an FM state. The ZB-type CrAs, which has been synthesized in the experiment,\textsuperscript{[20]} is 0.885 eV higher in energy than the MP-type AFM state, which agrees well with the former’s work.\textsuperscript{[37]} The equilibrium energy and volumes of the FM ZB-type and FM WZ-type are almost the same, with their difference being only 2 meV and 0.09 Å$^3$ per formula unit, respectively.

3.3. The Magnetic Properties of CrAs

CrAs in ZB, CC, WZ, and RS phases prefer the FM state. We calculated the magnetic moments of those four structures in the FM phase at different volumes, and the results are presented in Table 1 and Figure 2d. The magnetic moment for ZB-type and WZ-type CrAs in the FM state was calculated as 3 $\mu_B$ per CrAs pair at the equilibrium volumes, which is in excellent agreement with the saturation moments estimated experimentally\textsuperscript{[19]} and

Figure 1. Six types of crystal structures of CrAs. a) The cubic rocksalt (RS) structure; b) the cubic Csl (CC) structure; c) the cubic zinblende (ZB) structure; d) the hexagonal wurtzite-type (WZ) structure; e) the hexagonal NiAs-type (NA) structure; and f) the orthorhombic MnP-type structure.
3.4. The Electronic Properties of CrAs

To study the electronic structures of the CrAs system, the density of states (DOS) is calculated with optimized structures. MP- and NA-type CrAs are AFM metallic phases that have been studied in previous works. [6,10,16] Our calculations are consistent with previous works. In this article, we focus on the FM phase. Spin-resolved DOS of RS-, CC-, ZB-, and WZ-type CrAs in the FM state are presented in Figure 3. The Cr-d orbitals dominated the DOS around the Fermi level.

We defined the $E_{bc}$ and $E_{tv}$ as the bottom energy of minority-spin conduction bands and absolute values of the top energy of minority-spin valence bands with respect to the Fermi energy, respectively. The half-metallic (HM) gap is defined as the minimum of $E_{bc}$ and $E_{tv}$. ZB and WZ phases have a clear HM gap, which is essential to a half-metallic ferromagnet with 100% spin-polarized carriers. A large HM gap of 0.49 eV was founded in the WZ-type FM phase, which agrees with former work. [23,38] For the mechanism of HM in the ZB and WZ structures of CrAs, please see the Ref. [23,38,43].

Figure 3a displayed the DOS of RS-type CrAs. The DOS at the minority-spin channel is very small but not zero. The lack of HM gap around the Fermi level indicates that the RS-type structure is not half-metal. But spin polarization of RS-type CrAs at the fermi
level is high. In contrast with RS, ZB, and WZ structures, CC-type CrAs has a small spin polarization of 2.8% at the Fermi level.

3.5. The Optical Properties of CrAs

We further calculated the dielectric function to study the optical properties of CrAs. Since the CC-, ZB- and RS-type CrAs have isotropic lattices, only the results for the a-axis are presented. Considering the anisotropy lattice of MP, NA, and WZ structure, the results for the a-axis and c-axis (including the b-axis for MP) are displayed.

As shown in Figure 4a,b, the absorption coefficient $\alpha$ of NA-type CrAs in the infrared region (0.6–1.3 eV) is higher than that of other phases along a different axis. In the ultraviolet region (3.5–5 eV), the NA structure has a higher $\alpha$ along the a-axis, and the MP structure has a slightly higher $\alpha$ along the b-axis.

Based on Figure 4c,d, it can be seen that NA structure has a higher reflectivity $R$ in the infrared region (0.6–1.3 eV). The $R$ of NA structure along the c axis is 78.9% at 1.435 eV, which is significantly higher than other phases. In the visible-light region (1.64–3.19 eV), the $R$ of WZ and ZB structures along the a-axis is lower than in other phases, and there is no such phenomenon on the c-axis. And the $R$ of NA and MP structures along the a-axis in the ultraviolet region (3.5–5 eV) is significantly higher than in other phases.

The energy loss spectrum $L$ (as shown in Figures 4e,f) corresponds to the reflection coefficient $R$, and the position with the largest energy loss corresponds to the position where the reflection coefficient drops sharply. At about 1.8 eV, the reflection curvature of the NA structure along the c axis decreases, and the energy loss coefficient has a peak at the same energy position as shown in Figure 4d,f. Similarly, the reflection curve of CC and WZ structures drops about 3.0 and 1.8 eV along the a-axis as shown in Figure 4c,e, respectively. As a result, the energy loss coefficient has a peak at the same energy position.

Table 1. The lattice types (LT), space group (SG), magnetic state (MS), lattice constant $a$ (Å), length of Cr-as bond $L$ (Å), bulk module $B$ (GPa), magnetic moment per formula unit $M$ ($\mu_B$), cohesive energy $E_c$ (eV atom$^{-1}$), and relative energy to MP-type structure $E_m$ (eV). The abbreviations TW and OW represent this work and other works, respectively.

| Results | LT   | SG | MS    | $a/b/c$       | $L$    | $B$  | $M$  | $E_c$       | $E_m$   |
|---------|------|----|-------|---------------|--------|------|------|-------------|---------|
| TW      | MP   | 62 | AFM   | 5.571/3.498/6.27 | 2.5562 | 83.33| –    | –           | –       |
| OW$^{[8]}$ | MP   | 62 | AFM   | 5.577/3.573/6.129 | –      | –    | –    | –           | –       |
| OW$^{[9]}$ | MP   | 62 | AFM   | 5.637/3.445/6.197 | –      | –    | –    | –           | –       |
| OW$^{[10]}$ | MP   | 62 | NM    | 5.649/3.465/6.209 | –      | –    | –    | –           | –       |
| TW      | NA   | 194| AFM   | 3.779/5.323      | 2.5558 | 135.36| –    | –           | –       |
| OW$^{[11]}$ | NA   | 194| AFM   | 3.628/5.561      | –      | –    | –    | –           | –       |
| OW$^{[12]}$ | NA   | 194| NM    | 3.55/5.68        | –      | –    | –    | –           | –       |
| TW      | CC   | 221| FM    | 3.0003          | 2.598  | 147.62| 1.183| –           | –       |
| TW      | WZ   | 186| FM    | 4.000/6.497      | 2.518  | 68.65 | 3.000| –           | –       |
| OW$^{[13]}$ | WZ   | 186| FM    | 4.002/6.530      | –      | 68.4  | 3.000| –           | –       |
| TW      | RS   | 225| FM    | 5.121           | 2.560  | 94.86 | 2.931| –           | –       |
| TW      | ZB   | 216| FM    | 5.643           | 2.455  | 68.83 | 3.000| –           | –       |
| OW$^{[14]}$ | ZB   | 216| FM    | 5.659           | –      | 71.0  | 3.000| –           | –       |

Figure 3. Spin-dependent total densities of states (DOS, states/eV per formula unit) of the four FM CrAs in a stable magnetic state. Upper and lower parts of every panel are for majority-spin and minority-spin, respectively.
3.6. The Doping Effect on CrAs

At last, we investigated the effect of external doping on the structural and magnetic properties of CrAs.

First, we replaced a part of Cr atoms in CrAs with Ti atoms. The compound is expressed as Cr$_{1-x}$Ti$_x$As, where $x$ represents the concentration of Ti atoms. We calculated the energy of the Cr$_{1-x}$Ti$_x$As compounds in different structures and different magnetic states. We found that MP and NA structures still have lower energy than other structures. The phase diagram of the CrAs system is shown in the inset of Figure 5a, which is drawn based on the energy difference between the MP-type and the NA-type $\Delta E = E_{\text{MP}} - E_{\text{NA}}$. It is found that the ground-state crystal structure is the orthorhombic MP-type when the doping concentration $x$ is less than 0.12. However, the compound Cr$_{1-x}$Ti$_x$As prefers the hexagonal NA-type structure for $x > 0.12$. We have examined the MP-type and NA-type Cr$_{1-x}$Ti$_x$As compounds in different magnetic states. The energy–volume curve of $x = 0.125$ at which CrAs exhibit a NA structure. It is shown that the ground-state phase is the FM state. The electronic state calculation indicates that Ti-doped CrAs at $x = 0.125$ is a magnetic metal.

Then we replaced a part of As atoms in CrAs with Te atoms. The compound form is named as CrAs$_{1-x}$Te$_x$, where $x$ represents the concentration of Te atoms. We found that the compound CrAs$_{1-x}$Te$_x$ still maintained the orthogonal MnP-type structure as a ground-state structure but has a magnetic phase transition from AFM to FM at $x = 0.5$, as shown in Figure 5b. The electronic state calculation indicates that Te-doped CrAs at $x = 0.5$ is also magnetic metal. We noticed that doping concentration in CrAs have reached more than 50%,[26] so the structural and magnetic phase transition might be observed in future experiment and be applied in the spintronic devices.

4. Conclusion

We adopted the first-principles calculations to study the structural, magnetic, optical properties, and doping effect in six CrAs structures. We found that the FM state is energetically favorable for RS-, CC-, ZB-, and WZ-type structures, while the AFM state is energetically favorable for NA- and MP-type
structures. MP-type structure in AFM state is the ground-state structure for CrAs compound. The DOS shows that ZB- and WZ-type structures exhibit HM behavior with a bandgap in the spin-down channel. RS- and CC-type CrAs are not half-metal and have a large and small spin-polarization at the Fermi level, respectively. The optical properties show that NA-type CrAs has a higher absorption coefficient and reflectivity in the infrared region at all the axis. NA- and MP-type CrAs have a high absorption coefficient and reflectivity in the ultraviolet region along the a-axis. WZ- and ZB-type CrAs have a small absorption coefficient in the visible region. At last, we found that Ti-doped CrAs occur a structural phase transition from MP-type structure to NA-type one at a doping concentration of about $x = 0.12$. The Te-doped CrAs can maintain the MP-type structure and exhibit an AFM-to-FM magnetic phase transition at a doping concentration of about $x = 0.5$. We hope that these results can stimulate further interest in both theoretical and experimental research of the CrAs compound.

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Conflict of Interest

The authors declare no conflict of interest.

Data Availability Statement

The data that support the findings of this study are available from the corresponding author upon reasonable request.

Keywords

chromium arsenide, half-metallic, optical properties, phase transition

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