

First Principle Study of MC (M = Al, Ga and In) at Equilibrium and under Negative Stress

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The electronic and magnetic properties of the hypothetical compounds of MC (M = Al, Ga and In) are investigated by using first-principle calculations and pseudo potential plane wave self-consistent field method based on density functional theory. In order to find the most stable phase of MC (M = Al, Ga and In), we study them in zinc-blende (ZB), rock salt (RS), wurtzite and NiAs crystal structures. Comparison of the total energies of these compounds indicates that RS structure is the most stable crystal structure. Our calculations show that these compounds are metals in all of these structures. However, many of the nanospintronic devices are the heterojunctions of half-metals and semiconductors where the crystal structures of the layers that are grown on the semiconductors are the same as that of the semiconductors. Since most of the semiconductors have ZB structure, we investigate the electronic and magnetic properties of these compounds in this structure. It is also shown that although MC (M = Al, Ga and In) compounds are metals in ZB structure, they will find half-metal structure when relatively high negative stresses are applied over them. Therefore these compounds could be used in spintronic devices.

Keywords: Electronic band structure, Magnetic properties, Density functional theory, Half-metals

INTRODUCTION

Half-metallic ferromagnets have attracted many attentions because of their applications in the field of spintronic [1]. A half-metallic ferromagnet is a material with two different band structures for the majority spin (spin-up) and the minority spin (spin-down); for one of the spin states, the Fermi energy is in the conduction band and for the other the Fermi energy is in the gap [2,3]. Since de Groot *et al.* [4] noticed the existence of half-metallic ferromagnetism in NiMnSb, some half-metallic compounds have been found theoretically or experimentally. Half-Heusler and full-Heusler alloys such as CoMnSb [5], Co₂FeSi [6] and CoFeCrZ (Z = Al, Si, Ga and Ge) [7], metallic oxides such as CrO₂ [8], MS (M = Li, Na and K) [9], several materials in zinc-blende (ZB) structure such as CrAs, CrSb and MnAs [10-13] and TiTe in wurtzite (WZ) structure [14] are some of the materials that are approved to be half-metallic ferromagnets theoretically or experimentally.

Different compounds of carbon atoms and non-transition metals have recently been investigated. First, it is found that MC (M = Ca, Sr, Ba) that are the combinations of carbon atoms with two-valent metals are half-metallic ferromagnets [15]. Then, MC (M = Li, Na and K) were also found to be half-metals [16]. Although the combination of carbon with one- and two-valent metals are half-metals at their stable phase, their properties under stress should also be investigated because when one wants to grow them over semiconductors, up to few layers, the half-metal will have the same structure as the semiconductor. If the semiconductor has greater (smaller) lattice parameters than those of the half-metal, a negative (positive) stress will be applied over it that generates a larger (smaller) volume for half-metal than that of its stable phase. Changing the volume of a sample would change its band structure. As the band structure of a material changes, it may lose its half-metallicity. Dong and Zhao [17] considered MC (M = Ca, Sr and Ba) under stress and they found that, for example, SrC loses its half-metallicity at a pressure of 32 GPa.

In almost all of the studies about the effect of stress on the band structure, the sample is a half-metal at first (at its

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stable phase). Then, the volume or the amount of stress at which the half-metal would lose its half-metallicity is investigated. These kinds of researches encouraged us to find a way of changing volume to obtain a half-metallic material which is not a half-metal in its stable volume. Searching for the materials which are vulnerable to become half-metals under negative pressure and concerning this point that there is no any research on the combination of carbon atoms with three-valent metals motivated us to consider MC (M = Al, Ga and In) as our samples. We study them in different crystal structures and we find that their most stable crystal structure is the rock salt (RS) structure. However, we consider the electronic and magnetic properties of these compounds in ZB structure, which is the structure of the most of semiconductors. Our findings also confirm that these compounds are metal at their equilibrium volume in ZB structure. We change the volume gradually and consider the DOS diagrams until they turn out to half-metals at certain higher volumes. In order to expand the volume, one can put a few layers of these compounds on a semiconductor substrate that has approximately the same lattice constant as the lattice constant at which these compounds become half-metals. The results show that some semiconductors exist with this property.

COMPUTATIONAL METHODS

Our calculations were carried out on the basis of density functional theory [18,19] as accomplished in the Quantum-ESPRESSO simulation package. We employed PWscf code [20] of the package and solved Kohn-Sham equations self-consistently. The ultra-soft pseudopotential plane wave method with generalized gradient approximation [21] proposed by Perdew, Burke and Ernzerhof [22], was used in the exchange correlation interactions to simulate the electron-ion interactions. A kinetic Energy cut-off of 35Ry for wave function expansion and 350Ry for charge density and potential expansion were used. A mesh of $(12 \times 12 \times 12)$ k-points was used to sample the Brillouin zone.

RESULTS AND DISCUSSION

First we calculate the total energy as a function of volume for all of the ZB, RS, WZ and NiAs crystal

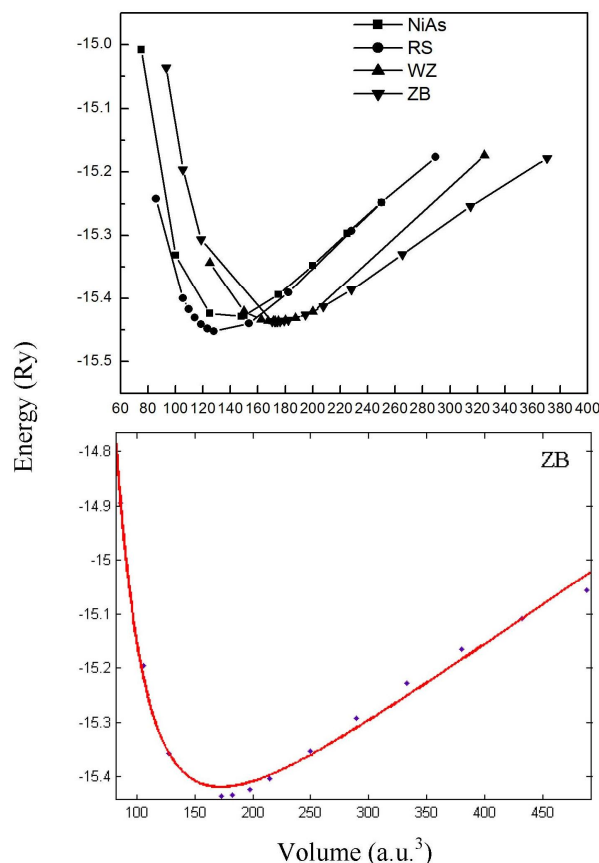


Fig. 1. Energy as a function of volume per formula unit for AlC in NiAs, RS, WZ and ZB crystal structures. The fit of the Murnaghan equation of state to the data points for ZB structure is also given at the bottom.

structures in order to find the most stable phase of MC (M = Al, Ga and In). Figure 1 shows the energy of AlC as a function of volume per formula unit; we do not show the similar figures for GaC and InC because they exhibit the same behavior in different crystal structures. As it is clear from this figure, the most stable phase is the RS structure. We calculate the lattice constants of these compounds in RS structure by fitting the total energy as a function of volume to the Murnaghan equation of state [23] and we find that the lattice constants at the stable phase are 4.11, 4.40 and 4.87 Å for AlC, GaC and InC, respectively. Although the most stable phase is the RS structure, we study these compounds in ZB structure because when we put a few layers of a compound over a substrate, for example by molecular beam

epitaxy (MBE) method, the structure of the compound is the same as that of the substrate [24]. Here we assumed that our substrate is a semiconductor in ZB structure, which is the structure of the most of semiconductors. The equilibrium lattice constants of AlC, GaC and InC in ZB structure are 4.68, 4.69 and 5.21 Å, respectively.

Next, we plot the density of states (DOS) and the band structures of these compounds at their equilibrium phase in ZB structure. Figure 2 represents the DOS diagram of AlC; we do not show the DOS diagram of GaC and InC since their DOS diagrams are approximately the same as that of the AlC. As seen in Fig. 2 and the similar figures, all these compounds are metals because the Fermi energy is in the conduction band for both spin-up and spin-down electrons.

Figures 3, 4 and 5 represent the band structures of AlC, GaC and InC, respectively, for the spin-up state; we did not show the band structure for the spin-down state because they are approximately the same as that of the spin-up state.

For a half-metal, the magnetic moment is an integer with respect to the Bohr magneton of an electron, μ_B ; we calculate the magnetic moment of MC (M = Al, Ga and In) as a function of lattice constant and look for lattice constants at which their magnetic moment are integers; Fig. 6 represents the results of our calculations for GaC.

We found that the magnetic moment of AlC, GaC and InC is $1 \mu_B$ at the lattice constants 5.87, 5.98 and 6.16 Å, respectively. We should plot the DOS diagram or the band structures to make sure that these compounds are half-metal at these lattice constants. Figures 7, 8 and 9 show their DOS, and as can be seen, all of them are half-metal at these lattice constants.

We also realize that, at these lattice constants, the energy of the ferromagnetic (FM) state is lower than that of the paramagnetic (PM) state (see Table 1). Therefore, they are more stable in the ferromagnetic state. This and our previous result approve that they are half-metallic ferromagnets at the lattice constant 5.87, 5.98 and 6.16 Å for AlC, GaC and InC, respectively. The semiconductors with almost the same lattice constant as these compounds are CdTe, ZnTe and GaAs that have lattice constants 6.48, 6.10 and 5.65 Å. It might be difficult to produce MC (M = Al, Ga and In) in these lattice constants because of the rather large difference between the lattice constants at which

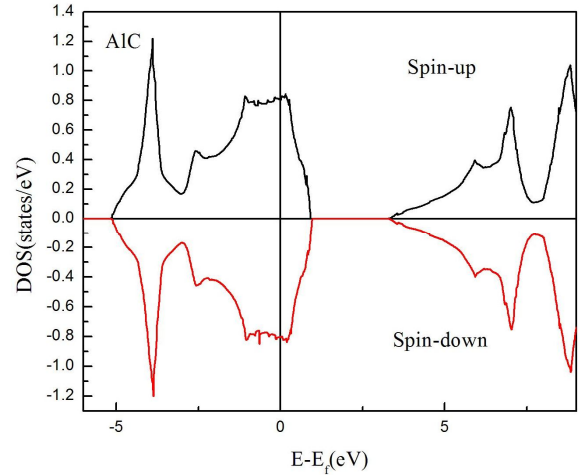


Fig. 2. DOS diagram of AlC at equilibrium.

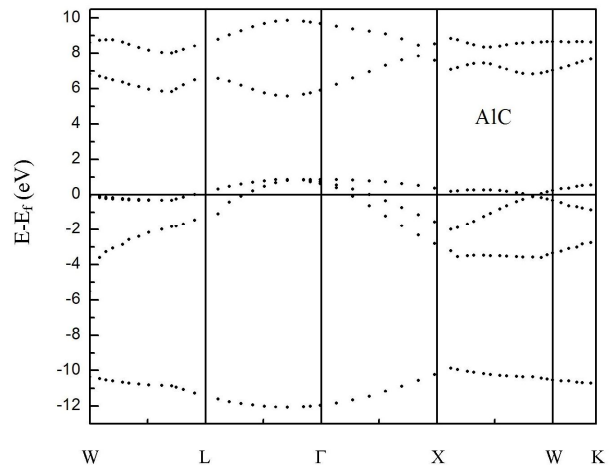


Fig. 3. The band structure of AlC.

they are half-metals and their stable phase ones, but we can modify this situation for example by inserting impurities [25].

CONCLUSIONS

The combinations of carbon atoms with one and two-valent metals have been previously investigated. Here we were interested to consider the electronic and magnetic properties of the combination of carbon atoms with three-valent metals. We chose MC (M = Al, Ga and In) as our

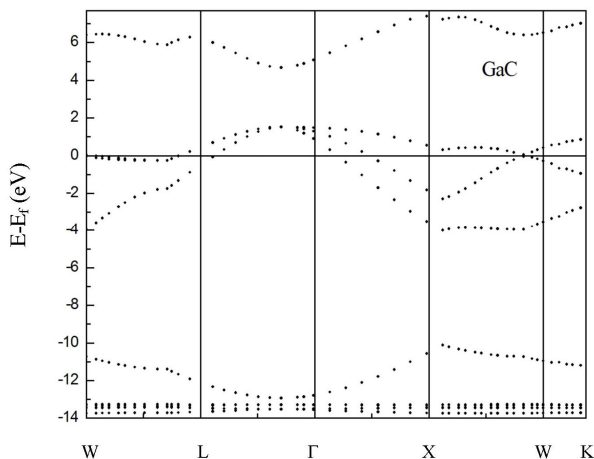


Fig. 4. The band structure of GaC.

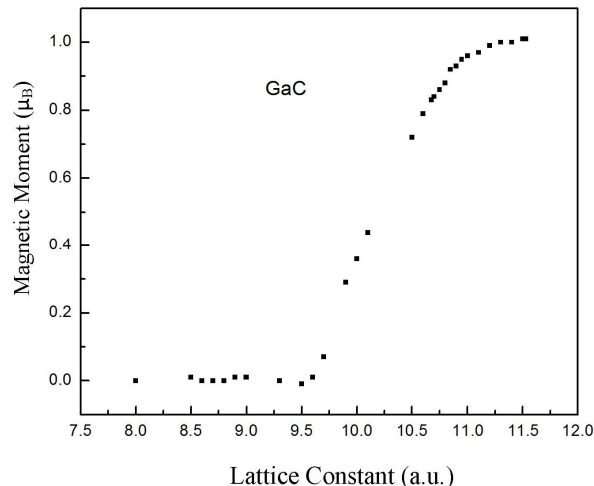


Fig. 6. Magnetic moment as a function of lattice constant for GaC.

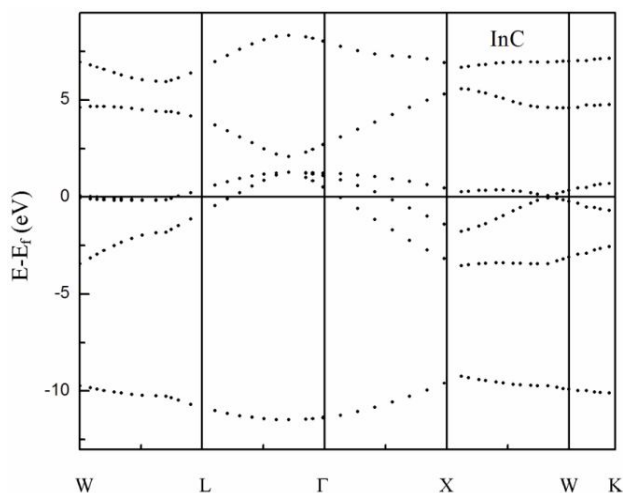


Fig. 5. The band structure of InC.

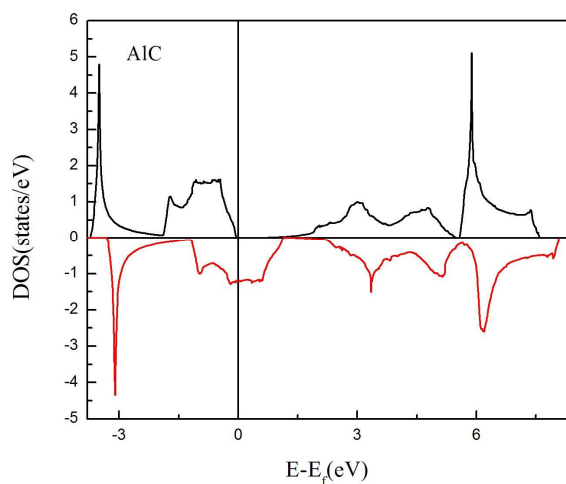


Fig. 7. The DOS diagram of AlC in the volume at which it has an integer magnetic moment.

samples. We found that the most stable crystal structures of these materials are the RS structures which are metals at their stable phases.

As we know, the material which is grown over a semiconductor should have the same crystal structure as the semiconductor up to few layers. Therefore, we have studied these compounds in ZB structure because most of the semiconductors have this structure. At the stable phase these materials show metallic behavior. Here, we found that MC (M = Al, Ga and In) become half-metal under negative

stress.

Certainly, the method of producing half-metals by applying negative stress is a new method of producing more diverse half-metallic compounds. Although producing MC (M = Al, Ga and In) in these lattice constants may be difficult because of the rather large difference between the lattice constants, we may succeed in producing them by modifying these compounds, for example by inserting impurities.

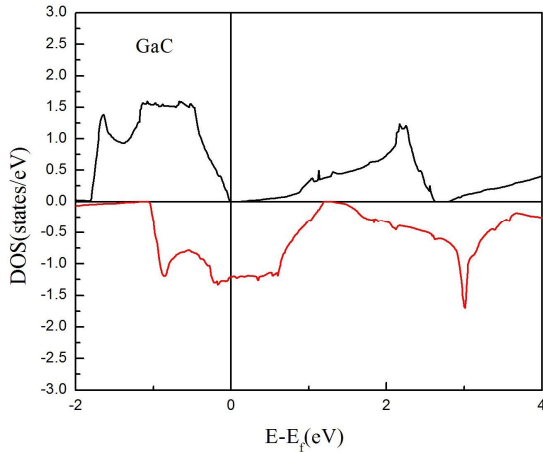


Fig. 8. The DOS diagram of GaC in the volume at which it has an integer magnetic moment.

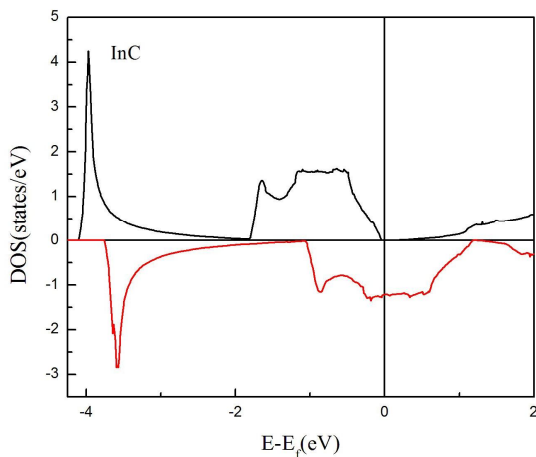


Fig. 9. The DOS diagram of InC in the volume at which it has an integer magnetic moment.

Table 1. Total Energies of MC (M = Al, Ga and In) in FM and PM Phases

Compound	Energy in FM phase (eV)	Energy in PM phase (eV)
AlC	-206.95	-206.90
GaC	-2569.72	-2569.68
InC	-1639.69	-1639.67

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