Improved half-metallic ferromagnetism of transition-metal pnictides and chalcogenides calculated with a modified Becke-Johnson exchange potential

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Abstract – We use a density-functional-theory (DFT) approach with a modified Becke-Johnson exchange plus local density approximation (LDA) correlation potential (mBJLDA) (semi-local, orbital-independent, producing accurate semiconductor gaps, see Tran F. and Blaha P., Phys. Rev. Lett., 102 (2009) 226401) to investigate the electronic structures of zincblende transition-metal (TM) pnictides and chalcogenides akin to semiconductors. Our results show that this potential does not yield visible changes in wide TM $d$-bands near the Fermi level, but makes the occupied minority-spin $p$-bands lower by 0.25–0.35 eV and the empty (or nearly empty) minority-spin $e_g$ bands across the Fermi level higher by 0.33–0.73 eV. Consequently, mBJLDA, having no atom-dependent parameters, makes zincblende MnAs become a truly half-metallic (HM) ferromagnet with a HM gap (the key parameter) 0.318 eV, being consistent with experiment. For zincblende MnSb, CrAs, CrSb, CrSe, or CrTe, the HM gap is enhanced by 19–56% compared to LDA and generalized gradient approximation results. The improved HM ferromagnetism can be understood in terms of the mBJLDA-enhanced spin exchange splitting.

Introduction. – It is believed that half-metallic ferromagnetic materials can be used to make high-performance spintronic devices [1,2], because one of their two spin channels is metallic and the other has the feature of a semiconductor or insulator, and then the spin polarization at the Fermi energy can reach 100% if the spin-orbit coupling effect is neglected [3]. Half-metallic ferromagnetism has been found in NiMnSb [3], CrO$_2$ [4], Fe$_3$O$_4$ [5], Co$_2$MnSi [6], and La$_{0.67}$Sr$_{0.33}$MnO$_3$ [7], and nearly 100% high spin-polarization has been observed experimentally in the cases of CrO$_2$ and La$_{0.67}$Sr$_{0.33}$MnO$_3$ materials [8]. It is of much interest to seek half-metallic ferromagnetic materials compatible with important semiconductors. Great efforts have been made in this direction, and significant progresses have been achieved in binary transition-metal pnictides and chalcogenides such as MnAs, MnSb, CrAs, CrSb, CrSe, and CrTe with zincblende [9–26] and wurtzite structures [27], special transition-metal–doped semiconductors [28,29], other transition-metal compounds based on convectional semiconductors [30–32] etc.

On the theoretical side, one usually uses the density-functional-theory (DFT) [33] method with generalized gradient approximation (GGA) [34], local density approximation (LDA) [35] etc. to study the electronic structures of these materials akin to semiconductors. Since it is well known that GGA and LDA underestimate semiconductor gaps, there naturally exists a question: how well do GGA and LDA describe the electronic structures of such half-metallic ferromagnetic materials? This needs to be answered because there exists some inconsistence between theoretical predictions and corresponding experimental observations. For examples, zincblende MnAs has been experimentally shown to be half-metallic [10–12], but both GGA and LDA calculations prove that it is not truly half-metallic [9] because the Fermi level touches or even crosses the bottom of the minority-spin conduction bands. Fortunately, there have already been many feasible approaches to improve DFT
calculations of semiconductor gaps, such as various GW methods [36,37], exact-exchange approach [38–40], different hybrid functionals [41], and a modified Becke-Johnson (mBJ) exchange potential [42]. Some of them demand high expenses in computational resources, and some are very economical. While being as computationally economical as GGA and LDA and needing no atom-dependent parameters, the mBJ exchange plus LDA correlation (mBJLDA) potential as an orbital-independent, semi-local exchange-correlation potential has been proved to produce accurate gaps for wide-band-gap insulators, sp semiconductors, and 3d transition-metal oxides [42]. Therefore, it is highly desirable, even necessary, to use this greatly improved, atom-parameters-independent, still economical DFT approach to investigate such half-metallic materials akin to semiconductors or insulators.

In this article we use a state-of-the-art DFT method with mBJLDA potential [42] to investigate the electronic structures of half-metallic ferromagnets akin to semiconductors. Our results show that in the cases of zincblende MnAs, MnSb, CrAs, CrSb, CrSe, and CrTe, mBJLDA does not yield visible changes in wide transition-metal oxides [42]. Therefore, it is highly desirable, even necessary, to use this greatly improved, atom-parameters-independent, still economical DFT approach to investigate such half-metallic materials akin to semiconductors or insulators.

In this article we use a state-of-the-art DFT method with mBJLDA potential [42] to investigate the electronic structures of half-metallic ferromagnets akin to semiconductors. Our results show that in the cases of zincblende MnAs, MnSb, CrAs, CrSb, CrSe, and CrTe, mBJLDA does not yield visible changes in wide transition-metal d-t_{2g} dominating bands near the Fermi level, but makes the occupied minority-spin p-dominating bands lower by 0.25–0.35 eV and the empty (or nearly empty) minority-spin e_{g} bands higher by 0.33–0.73 eV compared to GGA and LDA results. Consequently, mBJLDA makes zincblende MnAs become a truly half-metallic ferromagnet, being consistent with experiment, and enhances the half-metallic gaps [43] of the other five by 19–56%. The improved half-metallic ferromagnetism can be understood in terms of the fact that the spin exchange splitting is enhanced by using the mBJLDA potential. This consistency is a direct evidence that mBJLDA as a semi-local and orbital-independent exchange-correlation potential without atom-dependent parameters is very satisfactory in describing the electronic structures of such materials akin to semiconductors. More detailed results will be presented in the following.

The rest of the paper is organized as follows. We shall describe our computational detail in the next section. In the third section we shall present our main results calculated with mBJLDA in comparison with those calculated with the GGA and LDA. In the fourth section we shall make necessary discussions and try to understand the calculated results. Finally, we shall give our conclusion in the fifth section.

Computational detail. – We use a full-potential linearized augmented-plane-waves method within the density functional theory [33], as implemented in the package WIEN2k [44]. We use mBJLDA for the exchange-correlation potential [35,42] to do our main DFT calculations, and take popular LDA by Perdew and Wang (LDA-PW91) [35] and GGA by Perdew, Burke, and Ernzerhof (GGA-PBE) [34] to do corresponding comparative studies. The mBJ exchange potential [42] was developed from a semi-local exchange potential proposed by Becke and Johnson (BJ) [45]. The BJ exchange potential was developed from the Slater average of the Hartree-Fock potential [46]. It is required to satisfy invariance with respect to unitary orbital transformations, to have step-like structure in multi-shell atoms, to meet the exact uniform electron gas limit, and to exactly treat any (ground state) hydrogen-like atom, and thus can reproduce the shape of the exact-exchange optimized-effective potential of atoms [45]. The mBJ exchange potential is formulated by modifying the BJ potential by allowing the key BJ parameter to depend on the electron density and replacing the Slater average by Becke-Roussel potential because their difference is tiny [42,45,47]. mBJLDA as a combination of mBJ exchange and LDA correlation can produce accurate semiconductor gaps for sp semiconductors, wide-band-gap semiconductors, and transition-metal oxide semiconductors and insulators [42,48]. The full relativistic effects are calculated with the Dirac equations for core states, and the scalar relativistic approximation is used for valence states [49–51]. The spin-orbit coupling is neglected because it has little effect on our results. We use 3000 k-points in the first Brillouin zone, make harmonic expansion up to l_{max} = 10 in each of the atomic spheres, and set R_{mt} * k_{max} = 8. The radii of the atomic spheres of Mn, Cr, As, Sb, Se, and Te are set to 2.41, 2.41, 2.10, 2.27, 2.16, and 2.33 bohr, respectively. The volumes are optimized by using LDA-PW91 and GGA-PBE in terms of the total energy method. The self-consistent calculations are considered to be converged when the integration of the absolute charge-density difference between the input and output electron density is less than 0.0001 |e| per formula unit, where e is the electron charge.

Main calculated results. – At first, we investigate zincblende MnAs to show advantage of mBJLDA. This is because on the experimental side it has been shown to be half-metallic and intensively studied for device applications [10–12], but on the theoretical side both LDA and GGA calculations show that it is not truly half-metallic [9]. Since there is no corresponding energy functional for the mBJ exchange potential [42], we use experimental lattice constant as our computational input. We study its electronic structures by using the three exchange-correlation potentials: LDA-PW91, GGA-PBE, and mBJLDA. We present its total and partial DOSs calculated with mBJLDA, GGA-PBE, and LDA-PW91 in fig. 1. The mBJ result shows that zincblende MnAs is a half-metallic ferromagnet. The total magnetic moment per formula unit is 4\mu_B, in contrast with 3.86\mu_B calculated with GGA-PBE. The minority-spin gap across the Fermi level is 2.352 eV, substantially larger than the GGA-PBE result, 1.76 eV, and the half-metallic gap is determined by the bottom of the minority-spin conduction bands, being 0.318 eV. Similar results could be obtained by adding appropriate orbital-dependent on-site correlation...
parameters to some localized orbitals, as was done in the LDA+U approach [52] in the case of Co₂FeSi [53]. Another special feature in the mBJLDA DOS is that the As-p-dominating bands are merged with the Mn-d-dominating bands in the majority-spin channel, and the As-p-dominating bands in both spin channels are a little narrower than those calculated with both GGA-PBE and LDA-PW91. The mBJLDA DOS result implies 100% spin polarization at the Fermi level, but either LDA-PW91 or GGA-PBE result leads to much smaller spin polarization at the Fermi level. Therefore, the mBJLDA DOS is consistent with experiment, but either of the LDA-PW91 and GGA-PBE results is not.

In fig. 2 we present the spin-resolved energy bands between −5 and 4.5 eV of zincblende MnAs calculated with mBJLDA and GGA-PBE. There are little differences between mBJLDA and GGA for the majority-spin $t_{2g}$ bands near the Fermi level, but the mBJLFA raises the minority-spin $e_g$ bands by 0.3 eV and lowers the majority-spin $e_g$ bands by 0.3 eV. These are vital to make the zincblende MnAs become a truly half-metallic ferromagnet.

We present in fig. 3 the charge and magnetization density distributions of the zincblende MnAs calculated with the mBJLDA potential, within the charge density range 0.004–0.068 $|\rho|/\text{bohr}^3$ and the magnetization density $-0.008-+0.008|\mu_B|/\text{bohr}^3$, respectively. Here the energy range is from −5 eV to the Fermi level and the plane is
defined by the nearest As-Mn-As triangle. There is not any visible difference if mBJLDA is replaced by GGA. It can be seen that the Mn-As bond is covalent and there is a small negative magnetization around As although the total magnetic moment in the cell is contributed mainly by Mn.

The mBJLDA potential has similar effect on the electronic structures of other zincblende compounds, such as MnSb, CrAs, CrSb, CrSe, and CrTe. We present the spin-resolved total DOSs of zincblende MnAs, MnSb, CrAs, CrSb, CrSe, and CrTe calculated with GGA-PBE and mBJLDA. For the sake of comparison, we plot the GGA-PBE and mBJLDA DOSs in the same panel for each of the six zincblende compounds. It is clear that in each of the six cases the minority-spin gap across the Fermi level is made larger and the majority-spin $e_g$ bands move downward when GGA-PBE is replaced by mBJLDA. Furthermore, the bottom of the minority-spin conduction bands calculated with mBJLDA is higher than that with GGA, and consequently, the half-metallic gap is effectively made larger by replacing GGA with mBJLDA. All the mBJLDA results of the magnetic moments ($M$), the minority-spin gaps ($G_{\text{mis}}$), and the half-metallic gaps ($G_{\text{hm}}$) are summarized in table 1. For comparison, we also present the corresponding GGA-PBE results in the parentheses. It is clear that both $G_{\text{mis}}$ and $G_{\text{hm}}$ are made larger by replacing GGA-PBE with mBJLDA. Most importantly, zincblende MnAs is a truly half-metallic ferromagnet if mBJLDA is used. Therefore, the half-metallic ferromagnetism has been improved after we use mBJLDA instead of GGA-PBE.

Table 1: The lattice constants ($a$), magnetic moments per formula unit ($M$), minority-spin gaps ($G_{\text{mis}}$), and half-metallic gaps ($G_{\text{hm}}$) of zincblende MnAs, MnSb, CrAs, CrSb, CrSe, and CrTe calculated with mBJLDA. The values in the parentheses are calculated with GGA-PBE.

| Name  | $a$ (Å) | $M$ ($\mu_B$) | $G_{\text{mis}}$ (eV) | $G_{\text{hm}}$ (eV) |
|-------|--------|---------------|------------------------|------------------------|
| MnAs  | 5.717  | 4 (3.9)       | 2.352 (1.760)          | 0.318 (-)              |
| MnSb  | 6.166  | 4 (4)         | 1.923 (1.491)          | 0.459 (0.200)          |
| CrAs  | 5.659  | 3 (3)         | 2.579 (1.896)          | 0.636 (0.322)          |
| CrSb  | 6.138  | 3 (3)         | 2.180 (1.650)          | 0.992 (0.754)          |
| CrSe  | 5.833  | 4 (4)         | 4.569 (3.508)          | 1.331 (0.604)          |
| CrTe  | 6.292  | 4 (4)         | 3.692 (2.919)          | 1.384 (0.858)          |

**Discussions.** – It has been proved that the mBJLDA potential improves semiconductor gaps for various semiconductors [42]. Our calculated results have shown that the minority-spin gap across the Fermi level and the half-metallic gap (the key parameter [43]) of the binary transition-metal pnictides and chalcogenides are both improved by the mBJLDA potential. Especially, the nearly half-metallic zincblende MnAs under GGA and LDA becomes a truly half-metallic ferromagnet when we use the mBJLDA potential. This is consistent with the experimental result that zincblende MnAs is a truly half-metallic ferromagnet [10–12]. Therefore, we believe that the mBJLDA potential as an exchange-correlation potential is more satisfactory than both GGA and LDA in describing half-metallic ferromagnets akin to corresponding...

Fig. 4: (Color online) Spin-resolved density of states of MnAs (upper-left panel), MnSb (lower-left panel), CrAs (upper-middle panel), CrSb (lower-middle panel), CrSe (upper-right panel), and CrTe (lower-right panel) with the zincblende structure, calculated with mBJLDA (solid lines) and GGA-PBE (dashed lines), respectively. The upper part in each panel is for majority-spin channel and the lower part for minority-spin.
semiconductors, such as zincblende MnAs, MnSb, CrAs, CrSb, CrSe, and CrTe. More fortunately, the computational efficiency of mBJLDA is almost the same as those of GGA and LDA, and hence one can calculate large systems with mBJLDA as one does with GGA and LDA.

What causes this improvement? On the one hand, our calculated results show that replacing GGA with mBJLDA has little effect on the wide-majority-spin bands near the Fermi level. Actually, mBJLDA does not yield visible changes in wide transition-metal d-t2g bands with small density of states, but indeed shifts the narrow eg bands with respect to the t2g bands. We can see in fig. 4 that the occupied majority-spin eg bands emerge with the lower occupied majority-spin p-bands in the cases of MnAs and MnSb. On the other hand, the occupied minority-spin p-bands are lowered by 0.25–0.35 eV and the empty (or nearly empty) minority-spin eg bands are raised by 0.33–0.73 eV, which enhances substantially both the majority-spin gap and the half-metallic gap. These can be understood by assuming that it is the mBJLDA potential that enhances the spin exchange splitting with respect to GGA and LDA results. This explanation is supported by the observation in fig. 1 that there is much d-t2g weight at the top of the minority-spin valence bands and at the bottom of the minority-spin conduction bands. The enhancement of the spin exchange splitting is achieved because of the advantage of the BJ exchange potential [42,45]. Thus, the half-metallic ferromagnetism is enhanced in the binary transition-metal pnictides and chalcogenides akin to semiconductors.

**Conclusion.** – In summary, we have used a state-of-the-art DFT method with the mBJLDA potential [35,42] to investigate the electronic structures of zincblende transition-metal pnictides and chalcogenides and compare the mBJLDA results with those calculated with popular exchange-correlation potentials (GGA-PBE and LDA-PW91). Our calculated results show that the mBJLDA potential does not yield visible changes in wide transition-metal d-t2g bands near the Fermi level, but makes the occupied minority-spin p-bands lower by 0.25–0.35 eV and the empty (or nearly empty) minority-spin eg bands higher by 0.33–0.73 eV. In the cases of zincblende MnSb, CrAs, CrSb, CrSe, and CrTe, the half-metallic gaps are enhanced by 19–56% with respect to the GGA-PBE and LDA-PW91 results. Most importantly, the mBJLDA potential makes zincblende MnAs become a truly half-metallic ferromagnet. This result is consistent with experiment, which is a direct evidence that the mBJLDA potential is more satisfactory than popular GGA and LDA in describing the electronic structures of the binary transition-metal pnictides and chalcogenides akin to semiconductors. The improved half-metallic ferromagnetism can be naturally understood in terms of the enhanced spin exchange splitting caused by the mBJLDA potential. We believe that the semi-local and orbital-independent mBJLDA potential without atom-dependent parameters will be more satisfactory than usual GGA and LDA in calculating electronic structures with almost the computational efficiency of usual GGA and LDA for magnetic materials sharing some features with semiconductors.

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