

# Half-metallic ferromagnetism of MnBi in zincblende phase

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## Abstract

The full-potential augmented plane wave plus local orbitals method within density-functional theory is used to predict that MnBi in the zincblende phase is a true half-metallic ferromagnet with a magnetic moment of  $4.000\mu_B$  per formula. This phase of MnBi is found to be robust against volume changes from  $-12\%$  to  $+30\%$  and remains qualitatively the same under various exchange-correlation approximations.

*Key words:* half-metallic ferromagnetism; the zinc-blende MnBi; DFT

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## 1. Introduction

The half-metallic ferromagnet is a current hot topic and attracting more and more attention around the world, because it has a special band structure in which the minority-spin electrons are semiconducting while the majority-spin electrons keep the metallic character. This property makes it possible for them to play a key role in future electronic devices[1–3]. Since de Groot *et al* first predicted half-metallic ferromagnetism in Heusler compounds[4] in 1983, several half-metallic magnets, such as NiMnSb[5], CrO<sub>2</sub>[6], Fe<sub>3</sub>O<sub>4</sub>[7], have been theoretically predicted and experimentally found. Recently, the zincblende phase of MnAs and MnSb were predicted to be so-called ‘nearly half-metallic’ ferromagnetism, with full-potential density-functional calculations[8,9].

In this paper, the zincblende phase of MnBi was studied by the Vienna package WIEN2k[10] of the full-potential augmented plane wave plus local orbitals (FAPWLO) method within density functional theory[11] and predicted to be a full half-metallic ferromagnet with a magnetic moment of  $4.000\mu_B$  per

formula. The result is invariable when the volume changes from  $-12\%$  to  $+30\%$  and remains qualitatively the same under various exchange-correlation approximations. Although being meta-stable, this phase of MnBi could be grown epitaxially on appropriate substrates such as InSb or CdTe, for which the lattice mismatch is small. It comes as a new member in the family of half-metallic ferromagnets, and should be useful in spintronics and other applications.

## 2. Half-metallic ferromagnetism in the zincblende phase of MnBi

Using the zincblende structure but changing the lattice constant on a large scale, we found the zincblende MnBi to be a true half-metallic ferromagnet in a quite wide region of the lattice constant, and furthermore we obtained the optimized lattice constant. The density of states, energy bands, magnetic moments, and total energies are obtained for all lattice constants. Fig.1 is the spin-dependent density of states (SDOS) of the zincblende phase of MnBi with the optimized lattice constant 6.346 Å in GGA[12]. It is clear that the spin-up electrons are metallic but there is an energy gap of about 1.0 eV width at the Fermi energy in the bands of the spin-down electrons. The total SDOS around

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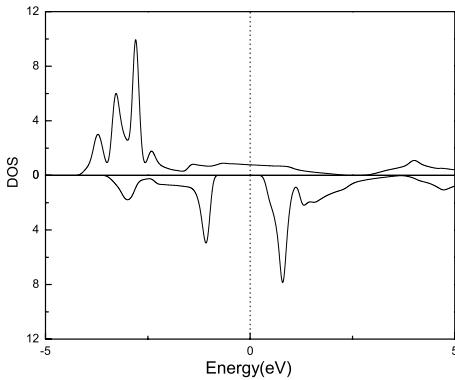


Fig. 1. The total DOS of MnBi in the zincblende phase with the optimized lattice constant 6.346 Å. There is a clear gap of approximate 1.0 eV width around the Fermi energy for the spin-down electrons.

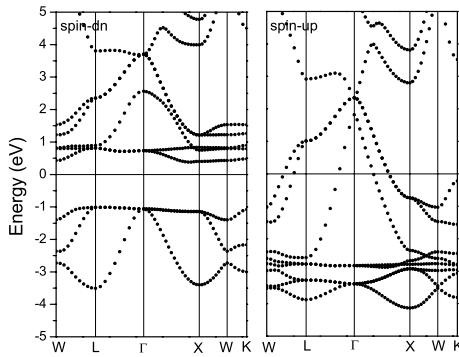


Fig. 2. Representative band structures of MnBi in the zincblende phase with the same parameters as Fig 1.

the Fermi energy consists mainly of the contributions of Mn  $t_{2g}$  and  $e_g$  and Bi  $p$  electrons and other electrons contribute little to the total SDOS. This means the zincblende MnBi to be a typical half-metallic ferromagnet. In Fig.2 we present the corresponding spin-dependent energy bands at high symmetry points in the Brillouin Zone. There are three bands crossing the Fermi energy. One of them is almost fully filled, but other two are approximately half-filled. The unfilled sections are around the  $\Gamma$  point for all the three bands. The total magnetic moment is  $4.000\mu_B$  per formula, also a typical character in half-metallic magnets. This is also in contrast with  $3.77\mu_B$  and  $3.75\mu_B$  per formula of the zincblende MnSb and MnAs[9]. Therefore, it is established by our accurate FAPWLO calculations that the zincblende MnBi is a true half-metallic ferromagnet.

In summary, we have studied the zincblende phase

of MnBi using the full-potential augmented plane wave plus local orbitals method within density-functional theory. The results of the density of states, energy bands, and magnetic moments clearly demonstrated that it is a typical half-metallic ferromagnet with a magnetic moment of  $4.000\mu_B$  per formula. This phase of MnBi is robust against volume changes from  $-12\%$  to  $+30\%$  and remains qualitatively the same under various exchange-correlation approximations. Although being meta-stable, it can be realized, at least as thin films or nanostructures through epitaxial growth on appropriate substrates of the important semiconductors such as InSb and CdTe, and should be useful in spintronics and other applications.

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