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Half-metallic properties of the $CuHg_2Ti$-type Mn_2ZnSi full-Heusler compound

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ABSTRACT

The half-metallic properties of novel $CuHg_2Ti$-type Mn_2ZnSi full-Heusler compound were examined by density functional theory (DFT) calculations. The electronic band structures and density of states of the Mn_2ZnSi compound show that spin-up electrons are metallic, but the spin-down bands are semiconductor with a gap of 0.48 eV, and the spin-flip gap is of 0.28 eV. The Mn_2ZnSi Heusler compound has a magnetic moment of 2 μ_B at the equilibrium lattice constant $a = 5.80$ Å. The Mn_2ZnSi full-Heusler compound is ferrimagnetic and maintains the half-metallic character having 100% polarization for lattice constants ranging between 5.62 and 6.91 Å.

1. Introduction

Spintronics is an emerging field in nanoscale electronics which uses the spin of electrons, rather than an electric charge, to encode and process data [1]. Half-metallic materials, in which one spin channel is metallic, while the other is semiconducting with an energy gap at the Fermi level, are highly attractive for spintronics applications because of their high spin polarization. This kind of materials showing a peculiar 100% spin polarization at the Fermi level have great attraction to scientific researchers due to the their potential device applications such as nonvolatile magnetic random access memories (MRAM) and magnetic sensors [2,3]. The concept of half metallic ferromagnets was first introduced by de Groot et al. [4], on the basis of band structure calculations in NiMnSb and PtMnSb semi-Heusler phases. So far, half metallic properties have been theoretically observed in many materials, for example ferromagnetic metallic oxides [5–7], dilute magnetic semiconductors [8,9] and zincblende transition-metal pnictides and chalcogenides [10–14]. The full-Heusler compounds have also been predicted theoretically to show half-metallic properties [15–21]. The full-Heusler compounds have attracted particular attention because they show a comparatively high Curie temperature and they are structurally similar to the widely used zinc-blende binary semiconductors such as GaAs and InP.

Recently, the first-principles calculations have been performed for the full-Heusler Mn_2ZnCa compound by Wang and Wei [22]. According to the their results, the Mn_2ZnCa compound is a half-metallic antiferromagnet with the band gap of 0.36 eV and half-metallic nature originates from the d–d orbital hybridization. Similar calculations based on density functional theory have also been carried out for the Mn_2CuSi compound [23]. The Mn_2CuSi compound is half-metallic ferrimagnet with the total magnetic moment of -1 μ_B. Although many Heusler compounds have been theoretically predicted to be half-metallic [15–21,24–28], the Mn_2ZnSi full-Heusler compound has never been investigated experimentally or theoretically up to now. In this paper, the electronic structure and magnetic properties of the Mn_2ZnSi full-Heusler compound with $CuHg_2Ti$-type structure are first studied by means of the self-consistent full potential linearized augmented plane wave (FPLAPW) method.

2. Computational method

Electronic structure calculations were performed using the self-consistent full potential linearized augmented plane wave (FPLAPW) method [29] implemented in WIEN2K code [30] within the density functional theory (DFT). The Perdew-Burke-Ernzerhof generalized gradient approximation (GGA) [31,32] was used for the exchange correlation correction. In this method the space is divided into non-overlapping muffin-tin (MT) spheres separated by an interstitial region. The muffin-tin sphere radii were 2.15 a.u. for Mn and Zn, 2.0 a.u. for Si. The convergence of the basis set was controlled by a cutoff parameter $R_{mt}K_{max} = 7$ where R_{mt} is the smallest of the MT sphere radii and K_{max} is the largest reciprocal lattice vector used in the plane wave expansion. The magnitude of

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the largest vector in charge density Fourier expansion (G_{max}) was 12. The cutoff energy, which defines the separation of valence and core states, was chosen as −6 Ry. We select the charge convergence as 0.0001e during self-consistency cycles. In these calculations, we neglected the effect of spin orbit coupling. For the Brillouin zone (BZ) integration, the tetrahedron method [30] with a 72 special k points in the irreducible wedge was used to construct the charge density in each self-consistency step.

3. Results and discussion

The Heusler compounds have a stoichiometric composition of X_2YZ, where X and Y are transition metals and Z is a main group element [33]. The X_2YZ Heusler compounds crystallize in the cubic $AlCu_2Mn$-type structure with the space group $Fm\bar{3}\ m$. In this structure, X, Y and Z atoms are placed on the Wyckoff positions 8c (1/4,1/4,1/4), 4a (0,0,0) and 4b (1/2,1/2,1/2), respectively. If the number of 3d electrons of Y atom is more than that of X atom, $CuHg_2Ti$-type structure with the space group $F\bar{4}\ 3m$ is observed. In this structure, X atoms occupy the nonequivalent 4a (0,0,0) and 4c (1/4,1/4,1/4) positions, while Y and Z atoms are located on 4b (1/2,1/2,1/2) and 4d (3/4,3/4,3/4) positions, respectively [17]. The calculated total energies versus volume are fitted to the empirical Murnaghan's equation of state [34] to determine the ground state properties. The calculated total energy as a function of lattice constant for both magnetic and non-magnetic configurations is plotted in Fig. 1 for the $CuHg_2Ti$-type structure. The computed lattice parameter, bulk modulus and its first derivative are $a = 5.80$ Å, $B = 138.665$ GPa and $B' = 5.220$, respectively. It can be seen that the magnetic phase has lower energy than paramagnetic phase. Up to now, an experimental or theoretical lattice constant value has not been reported.

In Fig. 2, we present the total and partial spin-polarized densities of states (DOS) of the Mn_2ZnSi compound at the equilibrium structure. It is clear that the majority-spin band is metallic, while the minority-spin band shows a semiconducting gap around the Fermi level. In minority-spin band, the valence band maximum is located −0.28 eV and the conduction band minimum at 0.20 eV. The energy gap for spin-down electrons at around the Fermi level is 0.48 eV. This energy gap in the minority-spin band gap leads to 100% spin polarization at the Fermi level, resulting in the half-metallic behavior at equilibrium state. The large exchange splitting of the Mn(1) and Mn(2) atoms causes the band gap around the Fermi level [35]. In the spin down band, the total density of states around the Fermi level are predominantly due to Mn(1)-d and Mn(2)-d electrons. The projected density of states of Mn atom lies mainly below the Fermi level and has the main contribution to the total DOS. The spin-down density of states of Mn(1) atom lies mainly below the Fermi level, while the spin-down density of states of Mn(2) atom lies mainly above the Fermi level. The energy region between −5.5 eV and −3.0 eV consists mainly of p electrons of Si atoms. The calculated total magnetic moment of Mn_2ZnSi compound is 2 μ_B, while the atomic magnetic moments are −0.741 μ_B for Mn (1), 2.596 μ_B for Mn (2), 0.020 μ_B for Zn and 0.032 μ_B for Si. The local magnetic moments of the manganese atoms are different from each other, indicating different atomic environments. The large bonding peak far below the Fermi level weakens the exchange splitting and reduces the magnetic moment of the Mn (1) atom. However, the Mn (2) atom is in a bcc crystal field, resulting in an e_g–t_{2g} splitting and a large spin moment. Similar behavior was also observed in the Mn_2NiSb and Mn_2CoZ (Z = Si, Ge, Sn and Sb) full-Heusler compounds [36,37].

The band structures of the Mn_2ZnSi at equilibrium geometry are plotted in Fig. 3. It is clear that the spin-up band structure has metallic intersections at the Fermi level which is sign of metallic

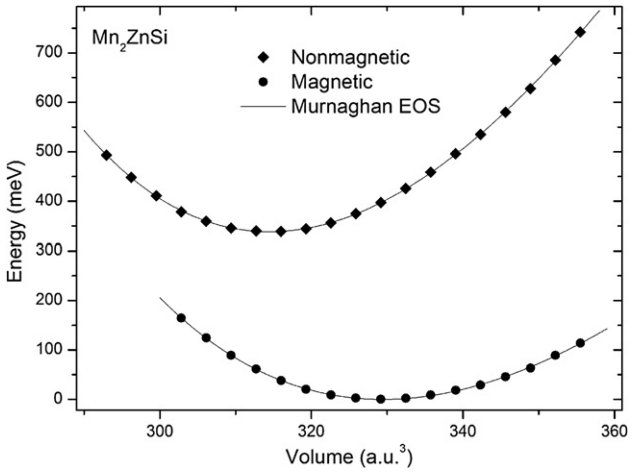

Fig. 1. The volume optimization for the Mn_2ZnSi Heusler compound.

nature. However, the spin-down band structure has energy gap at the Fermi level. The width of the energy gap can be calculated using the energies of the highest occupied band at the L point and the lowest unoccupied band at the L point. The Fermi level lies 0.28 eV

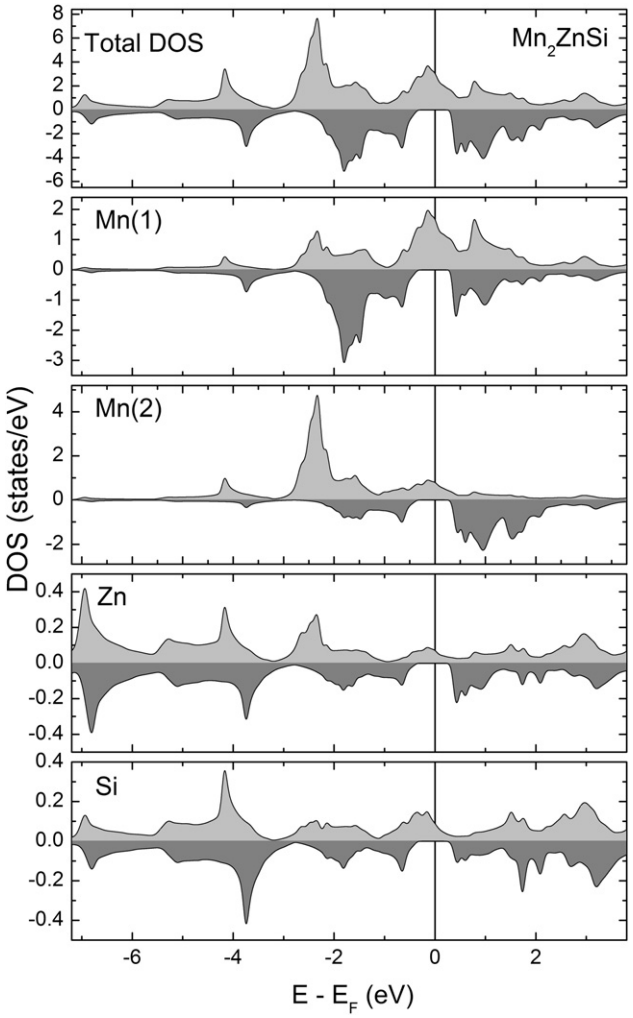

Fig. 2. The spin-polarized total densities of states (DOS) and atom-projected DOS.