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HEUSLER BASED FULLY COMPENSATED FERRIMAGNETIC SPIN GAPLESS SEMICONDUCTORS

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ABSTRACT

The spin-gapless semiconductors (SGSs) with a zero gap at the Fermi level in one of the spin channels, can make electrons easy to excite from the valence band to the conduction band with a small input of energy and simultaneously produce electron and hole carriers with 100% spin polarization. Recently, a new member of SGSs family, fully-compensated ferrimagnetic spin-gapless semiconductors (FCF-SGSs) have been predicted, they possess zero magnetization in addition to the properties of SGSs, which is an added advantage for practical application. Here, we study the Heusler-based materials with spin-gapless semiconducting behaviour, including half-Heusler compounds, full-Heusler compounds, and quaternary Heusler compounds.

Keywords: Spin-Gapless Semiconductor; Heusler Compounds; Slater-Pauling Rule.

I INTRODUCTION

Half-metallic ferromagnets (HMFs) [1], half-metallic fully-compensated ferrimagnets (HM-FCFs) [2], spin-gapless semiconductors (SGSs) [3], and fully-compensated ferrimagnetic spin-gapless semiconductors (FCF-SGSs) [4] have recently established considerable interest due to their advantages for applications in a number of novel spintronic devices. The energy band diagrams for these four kinds of materials are presented in Fig. 1.

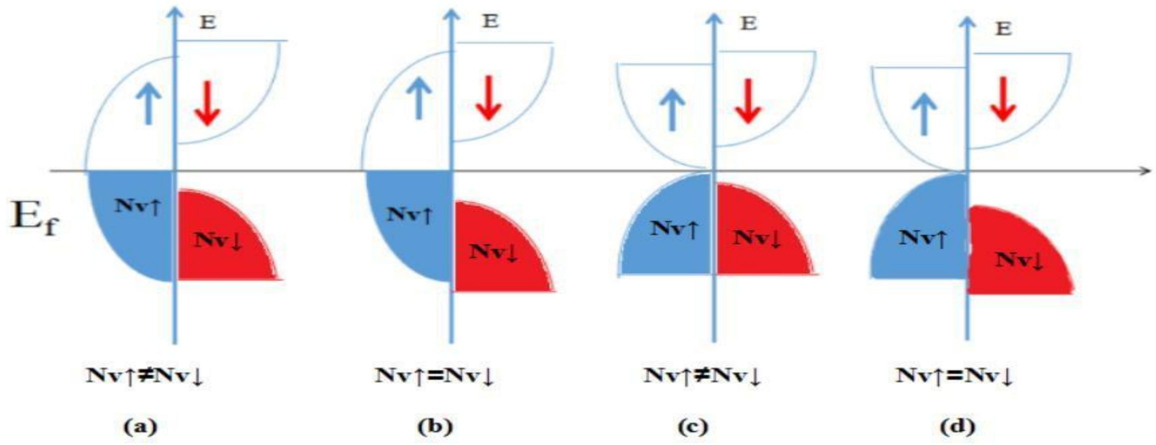


Fig. 1

As shown in Fig. 1a, half-metallic materials present metallic behavior for one spin channel and semiconductive behavior for the other spin channel, which results in a complete spin polarization of the conduction electrons at the Fermi level. As shown in Fig. 1b, a HM-FCF, also called a half-metallic antiferromagnet (HMAF) [5-8], is achieved when the number of majority spin ($N_V\uparrow$) and minority spin ($N_V\downarrow$) valence electrons are equal, i.e., $N_V\uparrow = N_V\downarrow$. In Fig. 1c, the SGSs, there is a zero gap at the Fermi level in the majority spin channel, in Fig. 1d, there is a special kind of SGS materials, called FCF-SGS, which will combine the properties of both an HM-FCF and a SGS. Here the number of spin-up valence electrons is equal to the number of the spin down ones ($N_V\uparrow = N_V\downarrow$).

Normally, there are two families of Heusler compounds, i.e., half-Heusler and full-Heusler. For the half-Heusler compounds XYZ, the sequence of sites is X-Y-void-Z, where X and Y are transition-metal elements and Z is an *sp*-element. The full-Heusler compounds [9, 10] have the chemical formula X_2YZ and are characterized by four interpenetrating face-centered cubic (*fcc*) lattices. Normally, when the valence of X is larger than that of Y, the Heusler compounds X_2YZ crystallize in the cubic space group Fm3 m (space group no. 225) with Cu_2MnAl ($L2_1$) as prototype, and the atomic sequence is X-Y-X-Z. When the valence of the Y element is the largest, the compounds crystallize in the so-called XA structure (also called the inverse structure), where the sequence of atoms is X-X-Y-Z and the prototype is Hg_2TiCu. Full-Heusler structure X_2YZ, is further extended into, DO_3-type X_3Z [11-15] and LiMgPdSn-type XMYZ [16-21]. DO_3-type X_3Z Heusler alloys have the *fcc* structure, and they have the same space group as the full-Heusler alloys X_2YZ. When X and Y are the same transition metal in Cu_2MnAl-type X_2YZ, it becomes DO_3-type X_3Z. In the DO_3 structure of X_3Z, the X (A) and X (C) atoms have the same neighboring environment, and they are surrounded by four X (B) and four Z atoms in a tetrahedral coordination [2]. (ii) LiMgPdSb-type Heusler compounds are quaternary compounds with the chemical formula XMYZ, where X, M, and Y are different transition metal atoms. The valence of M is lower than the valence of the X atoms, and the valence of the Y element is lower than the valence of both X and M. The sequence of atoms along the fcc cube's diagonal is X-Y-M-Z, which is energetically the most stable [10]. All the crystal structures of half-Heusler compounds, half-Heusler X_2Z compounds, full-Heusler X_2YZ compounds (XA and $L2_1$ types), DO_3-type compounds, and quaternary Heusler compounds are given in Fig. 2.

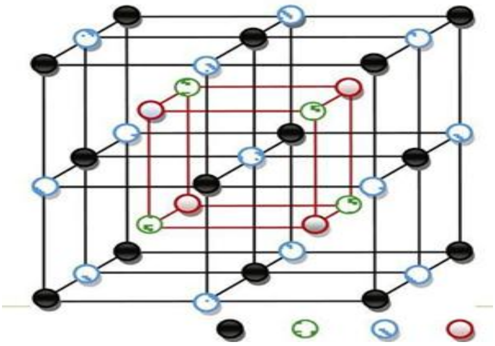
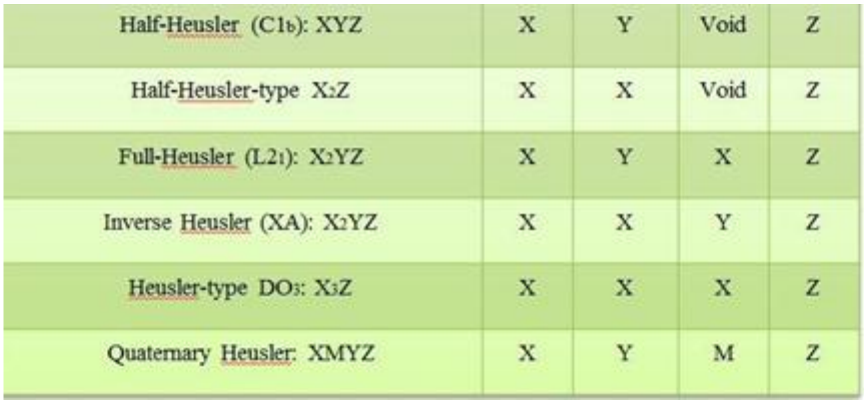


Fig.2



Half-Heusler ($C1_b$): XYZ	X	Y	Void	Z
Half-Heusler-type X_2Z	X	X	Void	Z
Full-Heusler ($L2_1$): X_2YZ	X	Y	X	Z
Inverse Heusler (XA): X_2YZ	X	X	Y	Z
Heusler-type DO_3: X_3Z	X	X	X	Z
Quaternary Heusler: XMYZ	X	Y	M	Z

We focus on Heusler based SGS materials and discuss about half-Heusler based SGSs, full-Heusler based SGSs, DO_3-type Heusler based SGSs, and LiMgPdSn-type quaternary Heusler based SGSs.

II Half-Heusler based SGSs

In half-Heusler XYZ, when X and Y are the same element in the half-Heusler structure (i.e., X = Y), a binary intermetallic compound X_2Z can be obtained [18, 19]. The structure of this type of compounds can be regarded as a special case of half-Heusler compounds with the $C1_b$-type structure. Recently, Zhang *et al.* showed that Mn_2Si [4, 20] is a potential candidate FCF-SGS. Mn_2Si compound can be regarded as a special case in the $C1_b$-type half-Heusler family. The electronic-structure calculated by Zheng *et al.* of Mn_2Si at its equilibrium lattice constant is displayed in Fig. 3. Obviously, as shown in Fig. 3, there is an indirect zero-width gap in the spin-up channel: the valence band maximum (VBM) of the spin-up electrons touches the Fermi level at the L-point. Both the conduction band minimum (CBM) of the spin-up electrons and that of the spin-down electrons touch the Fermi level at the X-point. Furthermore, the atomic magnetic moment of Mn (A) atoms is antiparallel to that of Mn (B), and the spin moment of the Z atom is negligible. The total magnetic moment of Mn_2Si is 0 μ_B. As shown in Fig. 3, nearly half of the spin-up states of Mn (A) are below the Fermi level, while most of the spin-down ones are above the Fermi level, reflecting a large exchange splitting, which leads to a net spin-down moment.

For the density of states (DOS) of Mn (B), most of the spin-up states are occupied, while half of the spin-down states are unoccupied, resulting in a net spin-up moment. The atomic environments of Mn (A) and Mn(B) atoms are different, and therefore, the configurations of the DOS of Mn (A) and Mn (B) are not same, which results in a partially compensated total DOS, but the total magnetic moment is fully-compensated

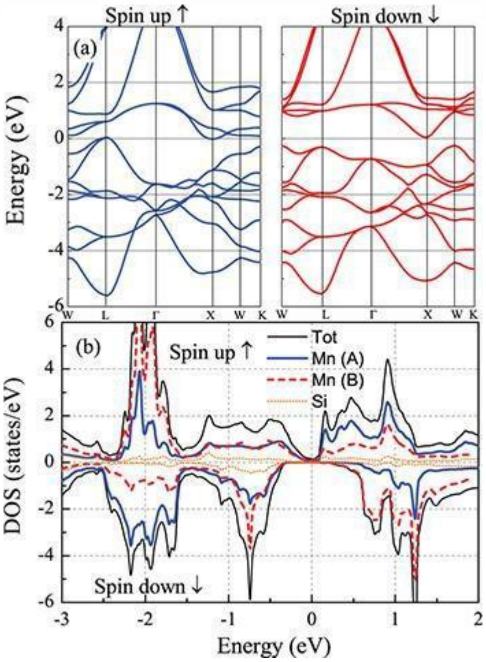


Fig.3

.III Full-Heusler based SGSs

Using first-principles calculations, the conditions for displaying spin-gapless conducting behavior in Mn_2CoAl compound were studied by Galanakis *et al.* [21] and Chen *et al.* [22]. By means of first-principles calculations, Skaftouros *et al.* [23] predicted the appearance of spin-gapless semiconducting behavior in Ti_2MnAl compounds. The calculated total magnetic moment of Ti_2MnAl compound is 0 μ_B, and thus, it can be classified as FCF. The band structures of Ti_2MnAl compounds with the inverse Heusler structure at their equilibrium lattice constants are displayed in Fig. 4. In the case of Ti_2MnAl, there is a direct zero-width band gap at the midpoint between the L and W high-symmetry points. Ti_2MnAl compound is a FCF-SGS, which combines the properties of a spin-gapless semiconductor, zero total spin moment, and a very high Curie temperature. , the FCF nature of Ti_2MnAl leads to the observation of small saturation magnetization, which is better from the viewpoint of application in spintronics devices.

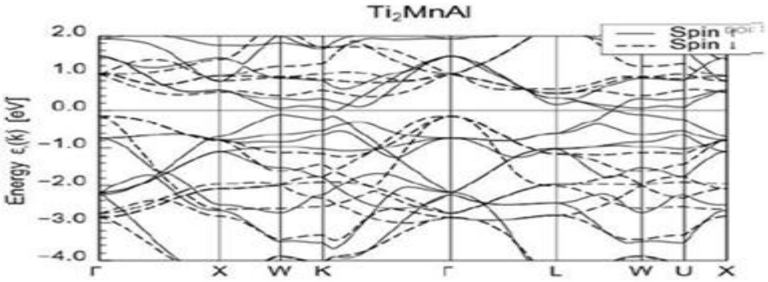


Fig.4

Recently, Wang and Jin [24] predicted that the fully-compensated ferromagnetic semiconductor (FCF-SM) Ti_2CrSi could achieve the FCF-SGS properties by lattice distortions. In their calculation work, two kinds of stran, i.e. uniform strain [25] and tetragonal distortion [26], have been applied to regulate and control the band gap. Jia *et al.* showed that the band gaps in the two spin channels of FCF-SM Ti_2CrSn can be adjusted to achieve the FCF-SGS nature by doping engineering. For FCF-SM Ti_2CrSn, the cases of substituting Si and Ge for Sn have been investigated in Jia *et al.*'s work [27]. The calculated results show that when Si or Ge is partly substituted for Sn in Ti_2CrSn compound the FCF behavior can be kept, while the band-gap width in the majority spin channel is continually narrowed down with increasing content of Si or Ge.

IV DO$_3$-type SGSs

V_3Al compound with the DO_3-type Heusler structure has only been investigated very recently. In 2013, Skaftouros *et al.* [23] proposed V_3Al compound, a DO_3-type Heusler alloy polymorph, to be FCF-SGS by employing *ab-initio* electronic structure calculations. The total and atomic DOS is shown in Fig.5. We can see that there is no energy gap in either the majority or the minority spin bands, which means that the gap for both the conduction and valence states vanishes at the Fermi energy. DO_3-type V_3Al compound can strictly be defined as an antiferromagnetic (AF) gapless semiconductor (GS). The AF gapless semiconducting DO_3 phase V_3Al was successfully synthesized via arc-melting and annealed following a process reported by Jamer *et al.* [28] in 2015.

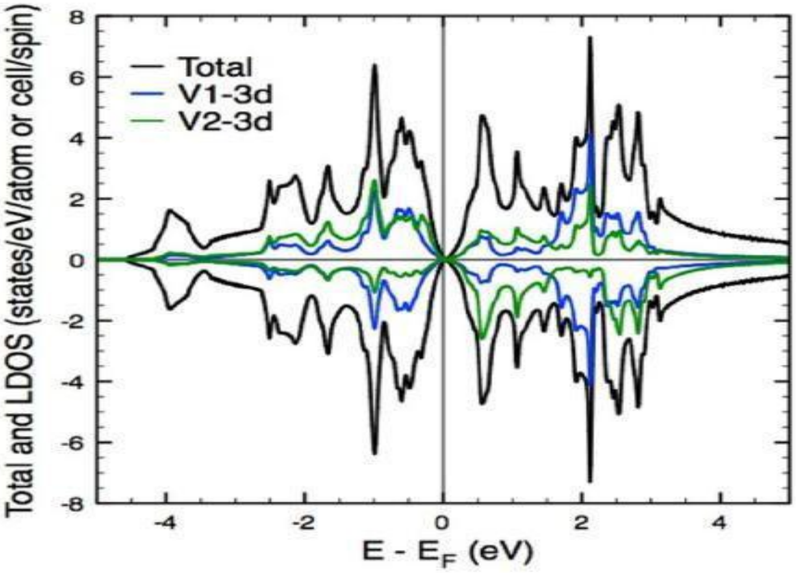


Fig.5

V LiMgPdSn-type quaternary Heusler based SGSs

Bainsla *et al.* [29] predicted a new SGS material, the equiatomic quaternary Heusler compound CoFeCrGa, from first-principle calculations, and then confirmed its SGS behavior experimentally. The DOS curves of CoFeCrGa at its experimental lattice constant (5.79 Å) and at strained lattice constants (5.71 Å, 5.60 Å, and 5.50 Å). In 2013, Xu *et al.* [28] investigated the band structures of the quaternary LiMgPdSn- Heusler compound CoFeMnSi by means of first-principle calculations. The calculated results showed that CoFeMnSi compound exhibits a unique electronic structure, characterized by a half-metallic gap in one spin channel, but a zero-width gap in the other spin channel, showing SGS behaviour. In 2015, by using structural, magnetization, spin-polarization magnetotransport, and Hall effect measurements, the SGS behaviour of CoFeMnSi was carefully confirmed experimentally by Bainsla *et al.* [30].

VI CONCLUSION AND OUTLOOK

The SGSs and FCF-SGSs are expected to open up many prospects for practical applications due to their unique electronic properties : 100% spin polarization with tunable charge-carrier concentrations and the generation of polarized photons. With potential applications in the spintronics, electronics, and optics fields, SGS has without a doubt become the topic of intense research in the condensed matter physics and materials science communities. More attention needs to be paid to the FCF-SGS materials, because these compounds will combine the properties of both a HM-FCF and a SGS. If this class of materials was used in spintronic devices, there would be no stray magnetic fields generated which usually exist in conventional MTJs with magnetic SFMs and might distort the domain structure of the magnetic material.

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