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Magnetic semiconductors based on quaternary Heusler compounds

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ABSTRACT

Based on Slater-Pauling rules a simple and effective semiempirical method for searching magnetic semiconductors were concluded. At the guild of this method magnetic semiconductors FeVNbAl, FeVNbGa, FeCrScSi, FeCrScGe, FeCrScSn, FeCrYSi, MnCrScSb, FeTiZrSb, MnVNbSn, FeVScSb, FeVYSb and CoVScSi were easily found. Band structure shows most of them are narrow bandgap semiconductors, and some are even close to spin gapless semiconductors. The maximal band gap is 0.373 eV found in FeVScSb, and the minimal band gap is 0.063 eV found in FeVNbGa. Those twelve new magnetic semiconductors well enrich magnetic semiconductor family and what's more this method may help other researchers to find more.

1. Introduction

The successful injection of spin-polarized current into a semiconductor has been expected for a long time in spintronics [1]. The most promising way to achieve it is spin filter materials (SFMs), which should be magnetic semiconductors [2]. Magnetic semiconductors can be simply classified to diluted magnetic semiconductors (DMSs) and concentrated magnetic semiconductors [3]. The DMSs such as $Ga_{1-x}Mn_xAs$ are usually made by introducing a high concentration of magnetic ions into semiconductors without magnetic. However, the DMSs are limited by their low Curie temperatures T_c, which is far more lower than room temperature [4]. Concentrated magnetic semiconductors are semiconductors with a periodic array of magnetic element [3]. Though the Curie temperatures of concentrated magnetic semiconductors like EuS and EuO even far low from DMSs [5], the simple mechanism and strong magnetic make them remain worth being researched.

Heusler compounds are famous for high T_c [6]. High T_c SFMs may exist in magnetic semiconductors based on Heusler compounds. Quaternary Heusler compounds have the most complex ingredient in the Heusler compounds, which means more possibilities. Many amazing performances have been found in quaternary Heusler compounds [7–11],which brings a research upsurge and shows us the wide spread application and special performance of them. It is reported several quaternary Heusler compounds such as CoFeMnZ (Z = Al, Si, Ga, Ge), NiFeMnGa, and NiCoMnGa exist Half-metallic ferromagnetism [12–15], which is quite close to magnetic semiconductors. Besides, the quaternary Heusler compounds CoVXAl (X = Ti, Zr, Hf) are reported to be ferromagnetic semiconductors with a Curie temperature considerably exceeding the room temperature [2].

Orbital hybridization theory is a useful tool to understand the property of alloys and predict new special performance alloys. To explain the origin of the energy gap, I. Galanakis analyzed how the full-Heusler alloys' orbital hybridized. They consider the energy gap comes from the orbital hybridization between A site atom and C site atom in the full-Heusler alloys with 24 valence electrons [16]. This rule can be extended to the quaternary Heusler compounds with 21 valence electrons for their similar structure, which is widely recognized [7,8]. If we just change the B site and D site elements in those compounds and keep the total number of valence electrons unchange, the band structure may change little. At the guide of this point and based on previous reported results [8], six new compounds are inferred. They are all still magnetic/spin-gapless semiconductors and keep similar energy band structure. Following this idea we find FeTiZrSb is also a magnetic semiconductor. Besides, according to the elementary periodic law, magnetic semiconductors FeVNbGa, FeCrScGe, FeCrScSn, FeCrYSi and FeVYSb are also found.

2. Computations detail and methods

First-principles calculations were performed using the CASTEP code based on the pseudopotential method with a plane-wave basis set [17,18]. The Perdew Burke Ernzerhof (PBE) functional of generalized

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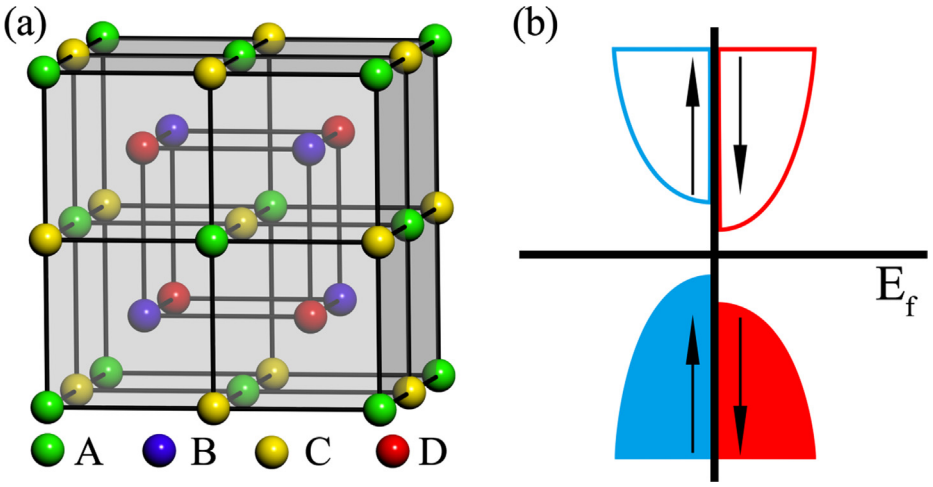

Fig. 1. (a) Schematic illustration of the Heusler compound. (b) Schematic energy band diagrams for a magnetic semiconductor.

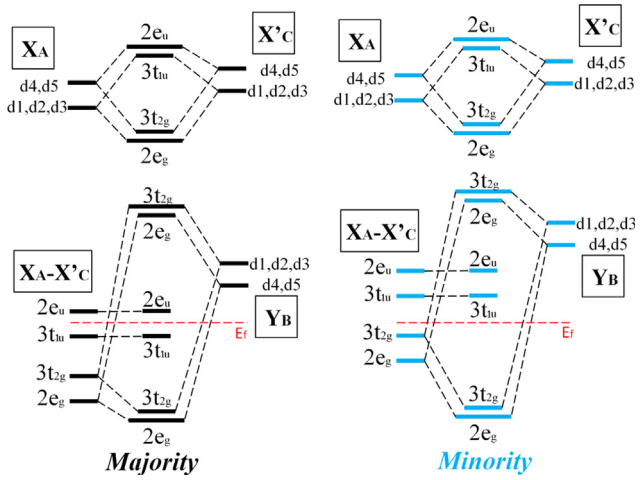

Fig. 2. Schematic representation of the energy levels of the majority and minority spin electronic band structure for the 21 valence electrons semiconductors.

gradient approximation (GGA) [19,20] was adopted for the exchange-correction functional. A Monkhorst-Pack grid with 283 summarized k points was used for Brillouin zone with a cutoff energy of 500 eV and a self-consistent field tolerance of 10^{-6} eV. To get the appropriate lattice constant, geometry optimization is prioritized.

3. Results and discussion

Fig. 1(a) shows schematic illustration of the Heusler compound. It can be decomposed into four interpenetrating fcc sublattices A, B, C, and D, which represents four kinds of site (A (0, 0, 0), B (0.25, 0.25, 0.25), C (0.5, 0.5, 0.5), D (0.75, 0.75, 0.75)). A quaternary Heusler compound XX'YZ has the space group of F-43m, and the four atoms occupy different sites separately. We call these compounds the LiMgPdSb-type compound because the structural prototype of the quaternary compounds is LiMgPdSb [21]. This structure has three possible nonequivalent superstructures. Type I: X is at A site, X' at B site, and Y at C site. Type II: X is at B site, X' at C site, and Y at A site. Type III: X is at C site, X' at A site, and Y at B site; the Z atom was fixed at D sites [22]. Lots of theory and experiment have proved type III is the

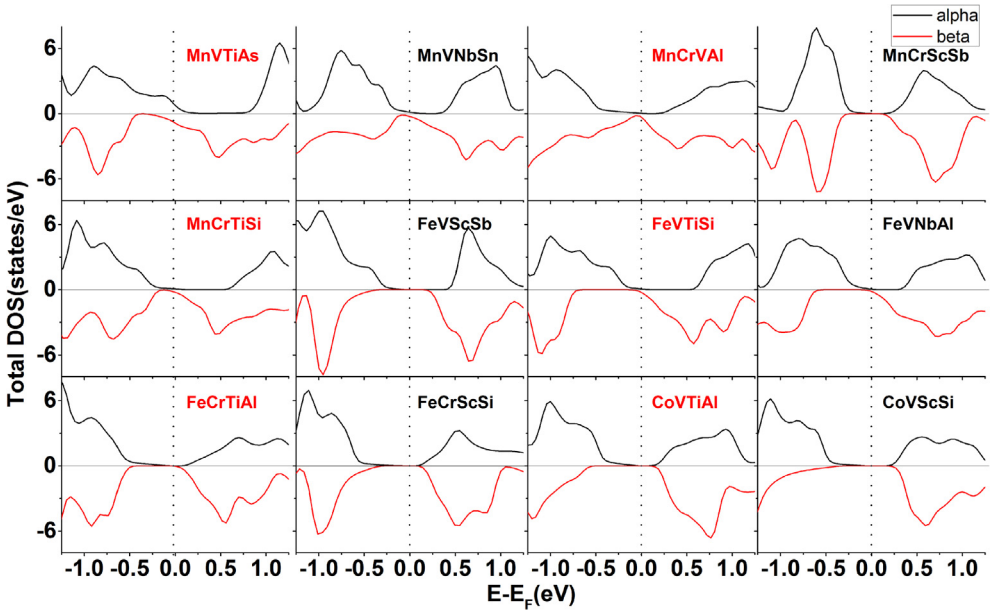

Fig. 3. Total DOS per formula unit for the compounds they calculated and we designed. Positive DOS values correspond to the spin-up states and negative DOS values to the spin-down states. The zero of the energy axis corresponds to the Fermi level.