

## ARTICLE

# First Principle Calculation of Electric and Magnetic Properties for New Half-metal $\text{Fe}_2\text{ScO}_4$

Jun Liu<sup>a,b\*</sup>, Xin-qiang Wang<sup>b</sup>, Yu Liu<sup>b</sup>, Hui-ning Dong<sup>b</sup>*a. College of Mathematics and Physics, Chongqing University, Chongqing 400030, China;**b. Institute for Applied Physics, Chongqing University of Posts and Telecommunications, Chongqing 400065, China*

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The new half-metals  $\text{Fe}_2\text{ScO}_4$  and  $\text{FeSc}_2\text{O}_4$  were designed and their spinel structures were optimized based on the first-principle pseudo-potential method. Their electric and magnetic properties including molecular magnetic moments and electronic structures were calculated and analyzed, and then were compared with those of  $\text{Fe}_3\text{O}_4$ . The calculation showed that  $\text{Fe}_2\text{ScO}_4$  and  $\text{FeSc}_2\text{O}_4$  were both new ferromagnetic II B-type half-metals, but  $\text{Fe}_3\text{O}_4$  was ferrimagnetic. The molecular magnetic moment of  $\text{Fe}_2\text{ScO}_4$  is about  $7.28 \mu_B$ , which is much larger than the  $4.0 \mu_B$  of  $\text{Fe}_3\text{O}_4$  and  $3.96 \mu_B$  of  $\text{Fe}_2\text{ScO}_4$ . The molecular magnetic moment of  $\text{Fe}_2\text{ScO}_4$  mainly came from the spin-polarization of Fe3d electrons. Also, the conductance of  $\text{Fe}_2\text{ScO}_4$  was a little larger than that of  $\text{Fe}_3\text{O}_4$ . For  $\text{Fe}_2\text{ScO}_4$ , the average electronic structure of Sc on A-sites was  $\text{Sc}^{+3} 3s^2 3p^4 3d^2$  and that of Fe on B-sites was  $\text{Fe}^{2+} t_{2g}^3 \uparrow t_{2g}^2 \uparrow t_{2g}^1 \downarrow$ . It can be predicted that the new half-metal  $\text{Fe}_2\text{ScO}_4$  has wider application ground in spin electronic instruments because of its larger magnetoresistance compared to  $\text{Fe}_3\text{O}_4$  and  $\text{FeSc}_2\text{O}_4$ .

**Key words:**  $\text{Fe}_2\text{ScO}_4$ ,  $\text{FeSc}_2\text{O}_4$ , Half-metal, Electronic structure, Molecular magnetic moment

## I. INTRODUCTION

It has been found recently that transmission of charges and spins of electrons may be simultaneously controlled in half-metals, which theoretically have 100% spin polarization of electrons at Fermi level [1-6]. If more dimensions are considered in magnetoresistance materials, more new applications will be proposed and more new spin electronic instruments will possibly be invented [7-14]. Therefore, it may be predicted that half-metal spin devices such as random-access memories, magnetic recording and writing head, magnetic sensors and spin transistors will have wider application ground than transition metal spin devices. To date, many half-metals such as  $\text{Fe}_3\text{O}_4$ ,  $\text{CrO}_2$ ,  $\text{FeCoS}_2$ ,  $\text{CuMnSb}$ ,  $\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3$ ,  $\text{Sr}_2\text{FeMoO}_6$ ,  $\text{Co}_{1-x}\text{Fe}_x\text{S}_2$ ,  $\text{Ti}_2\text{Mn}_2\text{O}_7$ , and  $\text{PdMnTe}$  have been found theoretically [8-19]. However, the room-temperature spin-polarization of these half-metals is often lower than 100% experimentally [18,19]. As a kind of II B-type half-metal, spinel  $\text{Fe}_3\text{O}_4$  has been found to have larger room-temperature spin-polarization and higher Curie temperature than other half-metals [18-21]. Therefore, spinel  $\text{Fe}_3\text{O}_4$  is thought to have more potential application than other half-metals. However, the room temperature magnetoresistance of multilayer films, granular films and powder films composed of  $\text{Fe}_3\text{O}_4$  is still not large enough to satisfy the demands of its application.

One of main reasons is that the conductance of  $\text{Fe}_3\text{O}_4$  is much lower than that of transition metals and their alloys, because Fe3d and Fe4s electrons are extremely localized by hybrid of Fe3d and O2p orbitals [22-25]. Another reason is that the molecular magnetic moment  $4.0 \mu_B$  of  $\text{Fe}_3\text{O}_4$  is too small so there is not enough spin-correlation scattering on transmitted electrons in  $\text{Fe}_3\text{O}_4$  in an applied magnetic field [18-22]. Therefore, it is necessary to probe new half-metal materials with larger conductance and molecular magnetic moment. Some research work has been carried on to improve electric and magnetic properties of the half-metal  $\text{Fe}_3\text{O}_4$ . For example, Chen *et al.* experimentally doped some Zn-ions into the half-metal  $\text{Fe}_3\text{O}_4$ , and then produced the new half-metal  $\text{Zn}_x\text{Fe}_{3-x}\text{O}_4$ . Moreover,  $\text{Zn}_x\text{Fe}_{3-x}\text{O}_4$  has much larger room-temperature magnetoresistance than  $\text{Fe}_3\text{O}_4$  [18]. Szotek *et al.* theoretically doped Co-ions or Ni-ions into  $\text{Fe}_3\text{O}_4$  and designed  $\text{Ni}_x\text{Fe}_{3-x}\text{O}_4$  and  $\text{Co}_x\text{Fe}_{3-x}\text{O}_4$ , and then carried on an *ab initio* study on charge order in  $\text{Ni}_x\text{Fe}_{3-x}\text{O}_4$ ,  $\text{Co}_x\text{Fe}_{3-x}\text{O}_4$ , and  $\text{Fe}_3\text{O}_4$  in detail. They found that both  $\text{Ni}_x\text{Fe}_{3-x}\text{O}_4$  and  $\text{Co}_x\text{Fe}_{3-x}\text{O}_4$  have half-metallicity [21,22].

In this work, Sc atoms were suitably doped into the half-metal  $\text{Fe}_3\text{O}_4$ , and Fe atoms on A-sites or on B-sites were replaced by Sc atoms. Then the geometrical structures of  $\text{Fe}_2\text{ScO}_4$  and  $\text{FeSc}_2\text{O}_4$  were both optimized based on the first principle pseudo-potential method, which is used effectively to design new materials and probe new properties of materials [26-35]. The electric and magnetic properties of  $\text{Fe}_2\text{ScO}_4$  were studied and compared with those of  $\text{Fe}_3\text{O}_4$  in system, and then the mechanisms were analyzed in detail.

\* Author to whom correspondence should be addressed. E-mail: liujun@cqupt.edu.cn

## II. MODEL AND METHOD

Geometrical structures of  $\text{Fe}_3\text{O}_4$ ,  $\text{Fe}_2\text{ScO}_4$ , and  $\text{Fe}_2\text{ScO}_4$  were optimized, and then their electric and magnetic properties were calculated based on the first principle pseudo-potential method. In the self-correction calculation, the k-point set was  $4 \times 4 \times 4$ . Their wave functions were expanded with plane-wave pseudo-potentials, and the exchange correlation functions used were the Perdew-Burke-Ernzerh functions (PBE) of three nonlocal gradient-corrected exchange-correlation functions (GGA). The cutoff energy was 340 eV.

An optimized primitive cell of  $\text{Fe}_2\text{ScO}_4$  is shown in Fig.1. There are 14 atoms including two Sc atoms on A-sites, four Fe atoms on B-sites and eight O atoms on other sites in a primitive cell. Fractional coordinates of the two Sc atoms are (0.125, 0.125, 0.125) and (0.875, 0.875, 0.875), respectively. Six 0.5-Fe atoms lie in the center of six faces (100) and one Fe-atom lies in the body center of the primitive cell. The crystal lattice constant and the crystal obliquity are 5.9355 Å and  $60^\circ$ , respectively. The volume is 147.858 Å<sup>3</sup> and the space group is m-3m. On the other hand, both  $\text{Fe}_3\text{O}_4$  and  $\text{FeSc}_2\text{O}_4$  have similar spinel structures of primitive cells. In the primitive cell of  $\text{Fe}_3\text{O}_4$ , all Fe atoms are on the A-sites and B-sites. In the primitive of  $\text{FeSc}_2\text{O}_4$ , two Fe atoms are on the A-sites and four Sc atoms are on the B-sites.

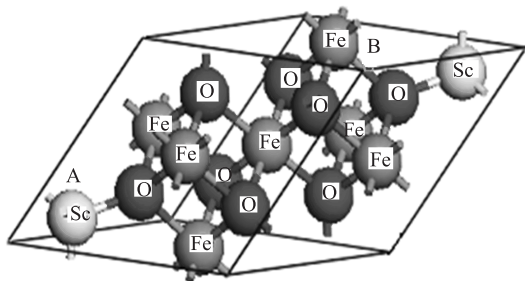


FIG. 1 An optimized primitive cell of the new half-metal  $\text{Fe}_2\text{ScO}_4$ , where the crystal lattice constant and the crystal obliquity are 5.9355 Å and  $60^\circ$ , respectively.

The total spin-polarized state densities of  $\text{Fe}_3\text{O}_4$  were calculated and are shown in Fig.2, where curves above and below the Fermi level correspond to up-spin and down-spin densities, respectively. From Fig.2,  $\text{Fe}_3\text{O}_4$  is a kind of B-type half-metal because there are only down-spin electrons at the Fermi level. These curves are basically in accord with experiments and those calculated by Szotek *et al.* [21,22].

Electronic charges and magnetic moments of all atoms in a  $\text{Fe}_3\text{O}_4$  primitive cell were calculated, as shown in Table I. In the table, the unit of spin is hbar and 1 hbar =  $2 \mu_B$ . From Table I, the magnetic moment 0.1  $\mu_B$  of an O-atom is very weak. The magnetic moments of Fe-atom on A-sites are  $-3.6 \mu_B$  and those of Fe

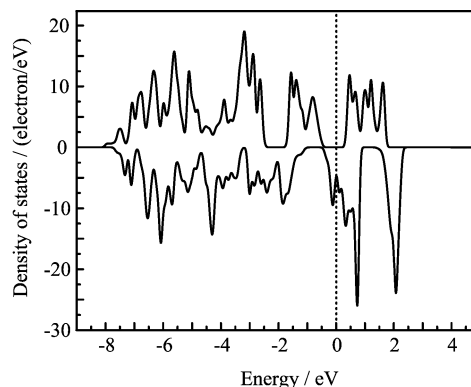


FIG. 2 The total spin-polarized state densities of  $\text{Fe}_3\text{O}_4$ .

atoms on B-sites are  $+3.6 \mu_B$ , which shows that  $\text{Fe}_3\text{O}_4$  is ferrimagnetic. The sum of magnetic moments of all atoms in a  $\text{Fe}_3\text{O}_4$  primitive cell is  $8.0 \mu_B$ . There are two molecules in an  $\text{Fe}_3\text{O}_4$  primitive cell, so the molecular magnetic moment of  $\text{Fe}_3\text{O}_4$  is  $4.0 \mu_B$ , which is equal to that calculated by Szotek *et al.* and basically agrees with the  $4.1 \mu_B$  obtained experimentally [21,22].

These results show that it is reasonable to optimize spinel structures of  $\text{Fe}_2\text{ScO}_4$  and  $\text{FeSc}_2\text{O}_4$ , and calculate their electric and magnetic properties based on the first principle pseudo-potential method.

TABLE I Electronic charges and magnetic moments of all atoms in a  $\text{Fe}_3\text{O}_4$  primitive cell

Atom	Electron in orbit			Total	Charge/e	Spin/hbar
	s	p	d			
O	1.86	4.85	0	6.71	-0.71	0.05
O	1.86	4.85	0	6.71	-0.71	0.05
O	1.86	4.85	0	6.71	-0.71	0.05
O	1.86	4.85	0	6.71	-0.71	0.05
O	1.86	4.85	0	6.71	-0.71	0.05
O	1.86	4.85	0	6.71	-0.71	0.05
O	1.86	4.85	0	6.71	-0.71	0.05
O	1.86	4.85	0	6.71	-0.71	0.05
Fe	0.31	0.50	6.20	7.01	0.99	-1.80
Fe	0.31	0.50	6.20	7.01	0.99	-1.80
Fe	0.35	0.53	6.21	7.08	0.92	1.80
Fe	0.35	0.53	6.21	7.08	0.92	1.80
Fe	0.35	0.53	6.21	7.08	0.92	1.80
Fe	0.35	0.53	6.21	7.08	0.92	1.80

In this work, the electric and magnetic properties of the half-metal  $\text{Fe}_2\text{ScO}_4$  are studied because the molecular magnetic moment  $7.14 \mu_B$  of  $\text{Fe}_2\text{ScO}_4$  is much larger than  $4.0 \mu_B$  of  $\text{Fe}_3\text{O}_4$  and  $3.96 \mu_B$  of  $\text{FeSc}_2\text{O}_4$ . Here the spinel structure of a  $\text{Fe}_2\text{ScO}_4$  primitive cell is optimized and the optimized positional parameters of atoms are compared with those not optimized. It was found that sites of Sc atoms and Fe atoms do not vary af-

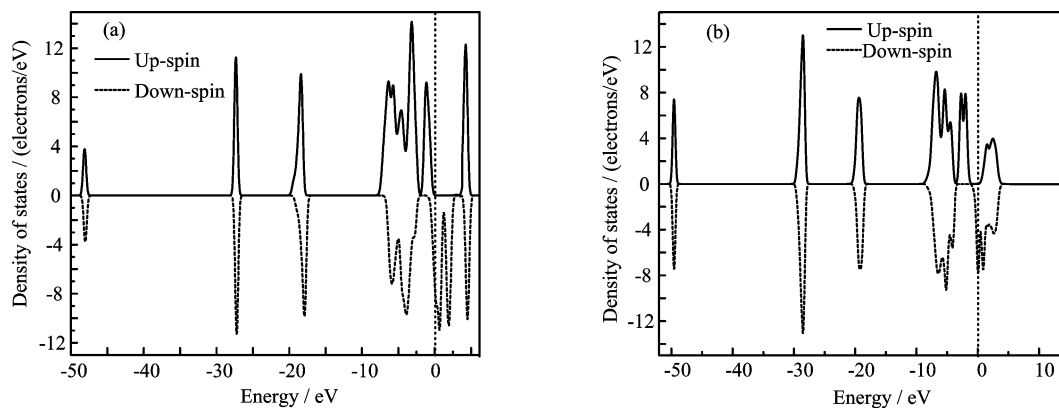


FIG. 3 Total spin-polarized state densities of half-metals  $\text{Fe}_2\text{ScO}_4$  (a) and  $\text{FeSc}_2\text{O}_4$  (b).

ter optimization, but O atoms all move a little toward Fe atoms. As an example, the fractional coordinate of one of two O atoms near Sc atoms varies from (0.2549, 0.2549, 0.2549) to (0.2581, 0.2581, 0.2581). Similarly, that of the other atom varies from (-0.2549, -0.2549, -0.2549) to (-0.2581, -0.2581, -0.2581). This shows that O-Fe covalent bonds are stronger in  $\text{Fe}_2\text{ScO}_4$  than in  $\text{Fe}_3\text{O}_4$ . The mechanism is that an Fe-atom has more 3d-electrons than one Sc-atom; hence there are stronger hybrid orbits of O2p and Fe3d than those of O2p and Sc3d in a  $\text{Fe}_2\text{ScO}_4$  primitive cell.

### III. RESULTS AND DISCUSSION

#### A. Total spin-polarized densities of states of $\text{Fe}_2\text{ScO}_4$ and $\text{FeSc}_2\text{O}_4$

Total spin-polarized state densities of  $\text{Fe}_2\text{ScO}_4$  and  $\text{FeSc}_2\text{O}_4$  were both calculated and are shown in Fig.3 (a) and (b), respectively. In Fig.3 real lines and dashed lines correspond to the up-spin sub-bands and spin-down sub-bands, respectively. From Fig.3, we can see there are only down-spin sub-bands at the Fermi level for both  $\text{Fe}_2\text{ScO}_4$  and  $\text{FeSc}_2\text{O}_4$ . Therefore,  $\text{Fe}_2\text{ScO}_4$  and  $\text{FeSc}_2\text{O}_4$  both have -100% spin-polarization at the Fermi level and they are both II B-type half-metals. This is similar to  $\text{Fe}_3\text{O}_4$ . However, both  $\text{Fe}_2\text{ScO}_4$  and  $\text{FeSc}_2\text{O}_4$  are approximately ferromagnetic according to our calculation that will be given later. This is different from ferrimagnetic  $\text{Fe}_3\text{O}_4$ . On the other hand, the state density 10.4 electron/eV of  $\text{Fe}_2\text{ScO}_4$  is much larger than the 7.5 electron/eV of  $\text{FeSc}_2\text{O}_4$  at the Fermi level. This shows that there are possibly more polarons to transit on B-sites in  $\text{Fe}_2\text{ScO}_4$  than in  $\text{FeSc}_2\text{O}_4$ , so  $\text{Fe}_2\text{ScO}_4$  possibly has larger conductance than  $\text{FeSc}_2\text{O}_4$  and  $\text{Fe}_3\text{O}_4$  [18]. From the definition of magnetoresistance  $MR = [R(H) - R(0)] / R(0) \times 100\%$ , the magnetoresistance of materials will be improved if their variation of resistance is enhanced and the zero magnetic field resistance is lowered. Therefore, the half-metal  $\text{Fe}_2\text{ScO}_4$

possibly has larger magnetoresistance than  $\text{FeSc}_2\text{O}_4$  [5,6,18].

#### B. Molecular magnetic moments of half-metals $\text{Fe}_2\text{ScO}_4$ and $\text{FeSc}_2\text{O}_4$

Electronic charges and magnetic moments of atoms in a  $\text{Fe}_2\text{ScO}_4$  primitive cell are shown in Table II. From Table II, the distribution of magnetic moment of atoms is  $0.34 \mu_B$  for an O-atom,  $0.14 \mu_B$  for an Sc-atom and  $3.76 \mu_B$  for an Fe-atom. Summing up all magnetic moments of 14 atoms, we can know the total is  $18.04 \mu_B$  for atoms of a  $\text{Fe}_2\text{ScO}_4$  primitive cell. The magnetic moment of covalent bonds were also calculated and shown in Table III. From Table III, there are  $0.04 \mu_B$  for one of eight O-Sc bonds,  $-0.1 \mu_B$  for one of 24 O-Fe bonds,  $-0.02 \mu_B$  for one of 24 O-O bonds and  $-0.20 \mu_B$  for one of six Fe-Fe bonds. Summing up magnetic moment of all bonds yields,  $-3.76 \mu_B$  from bonds of a  $\text{Fe}_2\text{ScO}_4$  primitive cell. Therefore the magnetic moment of a  $\text{Fe}_2\text{ScO}_4$  primitive cell is  $14.28 \mu_B$ . There are two molecules in one  $\text{Fe}_2\text{ScO}_4$  primitive cell so that the molecular magnetic moments of  $\text{Fe}_2\text{ScO}_4$  must be about  $7.14 \mu_B$ . Similar calculation carried out on  $\text{FeSc}_2\text{O}_4$  shows that the molecular magnetic moments of  $\text{FeSc}_2\text{O}_4$  total about  $3.96 \mu_B$ , which is much lower than the  $7.14 \mu_B$  of  $\text{Fe}_2\text{ScO}_4$ . If half-metals are in the same applied magnetic field, the larger molecular magnetic moments possibly result in stronger spin-correlation scattering for conductive electrons, and then larger variation of resistance. Therefore, it can be predicted that  $\text{Fe}_2\text{ScO}_4$  will have larger magnetoresistance than  $\text{FeSc}_2\text{O}_4$ , so in this work we focus on the electric and magnetic properties of the half-metal  $\text{Fe}_2\text{ScO}_4$ .

From Fig.3(a), for  $\text{Fe}_2\text{ScO}_4$  the number of up-spin electrons is equal to that of down-spin electrons when their energy is far lower than the Fermi energy. However, there is much difference between up-spin and down-spin state densities near the Fermi level. This shows that the large magnetic moments of  $\text{Fe}_2\text{ScO}_4$

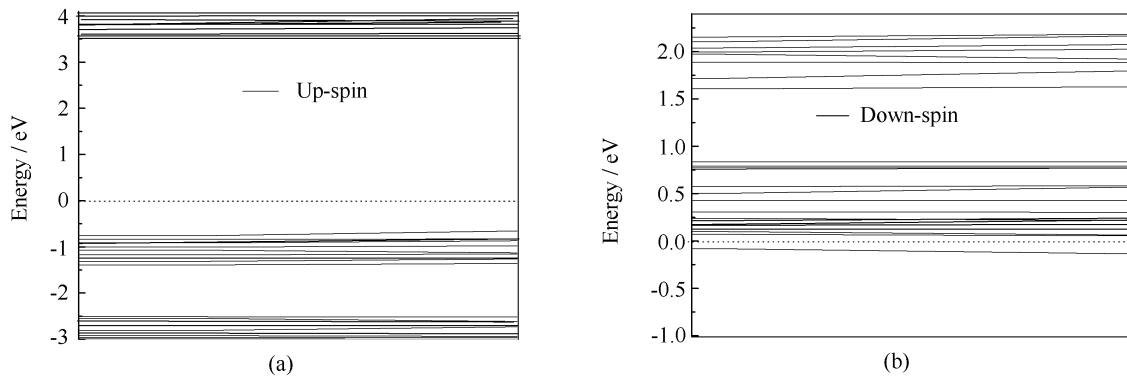


FIG. 4 Spin-polarized energy bands of  $\text{Fe}_2\text{ScO}_4$ , where (a) and (b) correspond to up-spin sub-bands and down-spin sub-bands, respectively.

TABLE II Electronic charges and magnetic moments of all atoms in a  $\text{Fe}_2\text{ScO}_4$  primitive cell

Atom	Electron in orbit				Charge/e	Spin/hbar
	s	p	d	Total		
O	1.85	4.91	0	6.76	-0.76	0.17
O	1.85	4.91	0	6.76	-0.76	0.17
O	1.85	4.91	0	6.76	-0.76	0.17
O	1.85	4.91	0	6.76	-0.76	0.17
O	1.85	4.91	0	6.76	-0.76	0.17
O	1.85	4.91	0	6.76	-0.76	0.17
O	1.85	4.91	0	6.76	-0.76	0.17
O	1.85	4.91	0	6.76	-0.76	0.17
Sc	2.13	6.2	1.39	9.72	1.28	0.07
Sc	2.13	6.2	1.39	9.72	1.28	0.07
Fe	0.33	0.53	6.26	7.12	0.88	1.88
Fe	0.33	0.53	6.26	7.12	0.88	1.88
Fe	0.33	0.53	6.26	7.12	0.88	1.88
Fe	0.33	0.53	6.26	7.12	0.88	1.88

TABLE III Calculated parameters of covalent bonds of  $\text{Fe}_2\text{ScO}_4$

Bond	Population/e	Spin/hbar	Length/Å	No. of bonds
O-Sc	0.50	0.02	1.93445	8
O-Fe	0.25	-0.05	2.03314	24
O-O	-0.04	-0.01	2.77651	12
Fe-Fe	-0.33	-0.10	2.96773	6
O-O	-0.05	-0.01	2.97081	12

come mainly from the spin-polarization of state densities near the Fermi level.

### C. Spin-polarized energy bands of $\text{Fe}_2\text{ScO}_4$

The spin-polarized energy bands of  $\text{Fe}_2\text{ScO}_4$  are shown in Fig.4, where (a) and (b) correspond to up-

spin sub-bands and down-spin sub-bands, respectively. From Fig.3, the down-spin sub-bands go through the Fermi level, but the up-spin sub-bands don't. This shows that there are only down-spin electrons at the Fermi level. However, as shown in Fig.4, there are no parabolas near the Fermi level. This shows that electrons at the Fermi level are extremely localized. On the other hand, we find the energy band curves of  $\text{Fe}_2\text{ScO}_4$  at the Fermi level are more acclivitous than those of  $\text{Fe}_3\text{O}_4$ , which are also calculated using a similar method. This shows the conductance of  $\text{Fe}_2\text{ScO}_4$  is a little larger than that of  $\text{Fe}_3\text{O}_4$ . Therefore,  $\text{Fe}_2\text{ScO}_4$  is a typical II-B half-metal with larger conductance than  $\text{Fe}_3\text{O}_4$ .

### D. Spin-polarized partial densities of states

Figure 5 shows the spin-polarized partial state densities of the new half-metal  $\text{Fe}_2\text{ScO}_4$ , where (a), (b), and (c) correspond to the s-orbits, p-orbits and d-orbits, respectively. The solid lines and the dashed lines correspond to the state densities of up-spin sub-bands and those of down-spin sub-bands respectively. The calculated electrons include those of  $\text{O}2s^22p^4$ ,  $\text{Fe}3d^64s^2$  and  $\text{Sc}3s^23p^43d^14s^2$ . In Fig.5(a), there are two main-peaks in the state density curves of s-electrons. The number of up-spin s-electrons is almost equal to that of down-spin s-electrons, so there is almost no spin-polarization for s-electrons. The first main-peak clearly comes from Sc3s electrons and the second main-peak mainly comes from some  $\text{O}2s^2$  electrons. Near the Fermi energy, there is a small quantity of Fe4s and Sc4s electrons. In Fig.5 (b) and (c), there is almost no spin-polarization for the  $\text{O}2p$  electrons about  $-28.0$  eV energy (in the third peak). Therefore, the peaks 1-3 have no contribution to the magnetic moments of  $\text{Fe}_2\text{ScO}_4$ . From the width of peaks 1-3, the above electrons are highly localized.

Comparing Fig.3 with Fig.5, we can conclude that the state densities near the Fermi level mainly come from hybrid orbits of  $\text{O}2p$  and  $\text{Fe}3d$  or  $\text{Sc}3d$ , which cor-

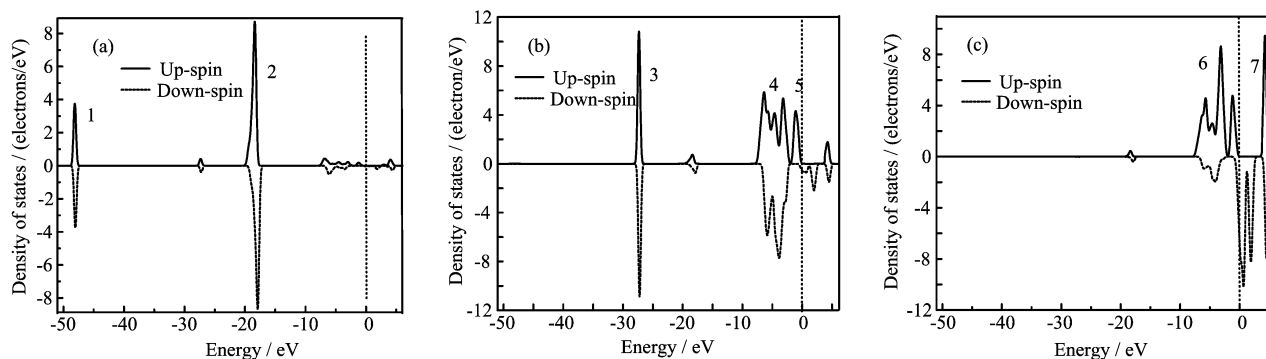


FIG. 5 Partial state densities of  $\text{Fe}_2\text{ScO}_4$ , where (a), (b) and (c) correspond to the s-orbits, p-orbits and d-orbits, respectively. The solid lines and the dashed lines up-spin sub-bands the down-spin sub-bands, respectively.

respond to main peaks 4 to 7. The number of up-spin p-electrons is a little larger than that of down-spin p-electrons, but the number of up-spin d-electrons is much larger than that of down-spin d-electrons. This shows that there is positive spin-polarization for the half-metal  $\text{Fe}_2\text{ScO}_4$  and the magnetic moments of  $\text{Fe}_2\text{ScO}_4$  come mainly from 3d-electrons. However, Table II shows that Sc3d electrons have little contribution for the molecular magnetic moments of  $\text{Fe}_2\text{ScO}_4$ .

### E. Electronic structure of $\text{Fe}_2\text{ScO}_4$

In order to analyze the electronic structure of  $\text{Fe}_2\text{ScO}_4$ , parameters of all atoms and covalent bonds in a  $\text{Fe}_2\text{ScO}_4$  primitive cell were calculated. Table II and III show the parameters of atoms and covalent bonds, respectively. The charges and the number of electrons including s-electrons, p-electrons, d-electrons and total electrons are given in Table II. Table III shows the parameters of covalent bonds including the charge population, the spins and the length of bonds.

From Tables II and III, the charges of an O-atom, an Fe-atom and an Sc-atom are  $-0.76$ ,  $0.88$  and  $1.28$  electrons, respectively. The charge number of covalent bonds is  $0.50$  electrons (e) for O–Sc,  $0.25$  e for O–Fe,  $-0.04$  e or  $-0.05$  e for O–O, and  $-0.33$  e for Fe–Fe. From the electronic charges of Sc atoms and the charge number of O–Sc bonds, some Sc4s electrons are transferred to O atoms, and other Sc4s electrons belong to both Sc atoms and O atoms because of Sc–O covalent bonds, which are caused by hybrid orbits of O2p and Sc3p or Sc4d. Furthermore, the calculated length  $1.93445$  Å for O–Sc bonds is shorter than that of other covalent bonds:  $2.03314$  Å for O–Fe,  $2.77651$  Å for O–O, and  $2.96773$  Å for Fe–Fe. This shows that O–Sc covalent bonds are very strong. Therefore, combining Table II and Fig.5, the electronic structure of the Sc-atom can be written as  $\text{Sc}^+3s^23p^43d^2$  and the number of up-spin electrons is equal to that of down-spin electrons approximatively. From Fig.5(c) and Table II, some Fe4s electrons are transferred to O atoms

and other Fe4s electrons belong to both Fe atoms and O atoms because of strong O–Fe covalent bonds, which are caused by hybrid orbits of O2p and Fe3d orbits. There are six Fe3d electrons including five up-spin electrons and one down-spin electrons. From theories of molecular orbits [18,22], it is concluded that there are four Fe3d electrons in  $t_{2g}$  orbits, where three electrons are up-spin and one is down-spin. Similarly, there are two up-spin Fe3d-electrons in  $e_g$  orbits in an Fe-atom. Therefore, the average electronic structures of Fe atoms can be approximated as  $\text{Fe}^{2+}t_{2g}^3t_g^2t_{2g}^\uparrow t_{2g}^\downarrow$ . In a word, magnetic moments of Sc atoms are very weak and those of Fe atoms are very strong so that  $\text{Fe}_2\text{ScO}_4$  is ferromagnetic. This is the reason why  $\text{Fe}_2\text{ScO}_4$  has much larger molecular magnetic moment than  $\text{Fe}_3\text{O}_4$ .

From Table III the length of O–Fe bonds is much shorter than that of Fe–Fe bonds. This shows O–Fe bonds are very strong, but Fe–Fe bonds are very weak, so most Fe3d electrons are localized, but a small quantity of electrons are itinerant. Therefore, the conductance of  $\text{Fe}_2\text{ScO}_4$  is a little higher than that of  $\text{Fe}_3\text{O}_4$ .

### IV. CONCLUSION

Based on these calculations,  $\text{Fe}_2\text{ScO}_4$  and  $\text{FeSc}_2\text{O}_4$  are both new ferromagnetic II-B-type half-metals, but  $\text{Fe}_3\text{O}_4$  is ferrimagnetic. The molecular magnetic moment of  $\text{Fe}_2\text{ScO}_4$  is  $7.14 \mu_B$ , which is much larger than the  $4.0 \mu_B$  of  $\text{Fe}_3\text{O}_4$  and  $3.96 \mu_B$  of  $\text{FeSc}_2\text{O}_4$ . The conductance of  $\text{Fe}_2\text{ScO}_4$  is a little larger than that of  $\text{Fe}_3\text{O}_4$ . There are hybrid orbits of O2p and Fe3d or Sc3d orbits near the Fermi level, which result in localization of Fe3d or Sc3d electrons of  $\text{Fe}_2\text{ScO}_4$ . It is predicted that  $\text{Fe}_2\text{ScO}_4$  has larger room-temperature magnetoresistance, and therefore wider application ground than  $\text{FeSc}_2\text{O}_4$  and  $\text{Fe}_3\text{O}_4$ .

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