Pnictide-height dependent ferromagnetism in CuFeAs and CuFeSb

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Electronic structures and magnetism properties of CuFeAs and CuFeSb are investigated by using first-principles calculations. We found that CuFeAs and CuFeSb share similar electronic structures and magnetic properties. Unlike the antiferromagnetic isostructure LiFeAs, the ground state of both compounds is ferromagnetic state driven by the Stoner ferromagnetic instability. Their ground state is very sensitive to the height of anion (As or Sb), translating from the ferromagnetic state to the stripe antiferromagnetic ordering when the anion height is smaller than a critical value. Such magnetic phase transition can be understood by the J_1 - J_2 Heisenberg model. Reducing the anion height will decrease the nearest-neighbor interaction J_1 but increase the next-nearest-neighbor interaction J_2 . The competing between the anion height dependent antiferromagnetic superexchange mediated by As(Sb) and the ferromagnetic direct exchange between Fe results the variations of magnetic structure with anion height.

Keywords: Superconductors, Electronic properties, Magnetic properties

I. INTRODUCTION

The emergence of superconductivity with high transition temperature (T_c) in ferropnictide¹⁻⁶ and ferrochalcogenide⁷⁻¹⁰ is helpful for understanding the mechanism of high- T_c Superconductors. The similar phase diagram to copper oxides, where superconductivity develops when magnetic order is destroyed by doping or high pressure, suggests a strong interplay between superconductivity and magnetism^{11,12}. It is generally accepted that the superconductivity in iron based superconductors is dominated by magnetism-mediated rather than phonon-mediated pairing. Therefore, it is important to study the mechanism of magnetism in Fe-based superconductors. To understand the magnetism puzzle, the scenarios based on both itinerant weak-coupling picture and the localized strong-coupling picture have been constructed. In the first picture, the magnetism can be understood by the Fermi surface (FS) nesting^{11,13-15}. However, this picture failed to explain the double-stripe antiferromagnetic (AF)¹⁶ ground state of FeTe, whose FS topology is similar to iron pnictides¹⁷. In the localized strong-coupling picture, the magnetic order is explained by the frustrated super-exchange interactions and the Heisenberg model for local spin moments¹⁸⁻²². Nevertheless, this model can not explain the metallic resistivity and is incompatible with the large anisotropy of the nearest-neighbor exchange constant²³. Apart from the above opposite viewpoints, a new theory with coupling the local moments and itinerant electrons has also been considered by Johannes²⁴ and Yin²⁵.

By first-principles calculations, Xu *et al*²⁶ presented a doping-dependent phase diagram of the LaOMAs ($M = V-Cu$) family, and found that the Fe-based compound was at the borderline between the AF and ferromagnetic (FM) phase regions. Yin *et al*²⁵ unified the FM and AF interactions in the microscopic model, where they assume that the superexchange AF interaction competes with the orbital-degenerated double-exchange FM interaction. With the increment of the anion height from the iron plane (Z_{anion}), the magnetic ground state evolve from the stripe AF order to the double-stripe AF order, and finally to the FM order. Moon's²⁷ calculations on $FeTe_{1-x}Se_x$ demonstrated that its ground state switched between stripe AF and double-stripe AF order with varying Z_{anion} , they also found the tendency toward FM state if the value of Z_{anion} was large enough.

Recently, two new layered ferropnictide compounds with formula as CuFeAs^{28,29} and CuFeSb³⁰ were synthesized, with their structures being similar to the layered tetragonal 111-type iron-based superconductors LiFeAs³ and NaFeAs⁴. The anions height is $Z_{As} = 1.74$ (1.81) Å in CuFeAs^{28,29} and $Z_{Sb} = 1.84$ Å in CuFeSb³⁰, which is significantly larger than $Z_{anion} = 1.31, 1.35, 1.51, 1.47$, and 1.73 Å in LaOFeAs¹, BaFe₂As₂², LiFeAs³, FeSe⁷ and FeTe⁸, respectively. Using magnetization and neutron scattering measurements, Qian *et al*³⁰ discover that the ground state of CuFeSb is metallic FM state. The magnetic properties of CuFeAs is under debate: Qian *et al*²⁹ reported that its ground state was FM, while Thakur *et al*²⁸ claimed the AF state. Until now, no first-principle calculations about CuFeAs and CuFeSb have been reported. In this paper we employed the first-principles technique to investigate the electronic structures and magnetism of these compounds.

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FIG. 1: (Color online) The DOS and projected DOS of (a) CuFeAs and (b) CuFeSb in the NM configure, with GGA formula.

II. METHODOLOGY

The calculations were performed by using STATE³¹ code based on the density functional theory (DFT). The generalized gradient approximation (GGA)³² with the Perdew-Burke-Ernzerhof (PBE)³³ formula for the exchange-correlation potentials was used in the calculation. All the lattice constants and atomic positions of both compounds were taken from experiments^{28,30}. To determine the true ground state, we considered four different cases: nonmagnetic (NM), FM, and the two AF spin configurations. The first one is AF1 (checkerboard AF), where the nearest-neighbor Fe spins are antiparallel in the a-b plane and ferromagnetic along the c-axis. The second one is AF2 (stripe AF), where the Fe spins along the square diagonal are aligned antiferromagnetically. The same unit cell was used for the NM, FM, and AF1 states, while we considered the unit cell as $\sqrt{2}a \times \sqrt{2}a \times c$ for the AF2 state. After carefully examining the convergence with respect to the cutoff energy and number of k-points, we adopted a cutoff energy of 30 Ry and the Monkhorst-pack k-points generated with $20 \times 20 \times 16$ grids for the NM, FM and AF1 states and $16 \times 16 \times 12$ grids for the AF2 state.

III. RESULTS AND DISCUSSION

Fig. 1(a) shows the density of states (DOS) and projected DOS of CuFeAs in the NM state. The Cu-3d states mainly lie between -5.0 and -2.0 eV, accompanying with the empty 4s state above the Fermi level (E_F). Therefore, the Cu 3d orbitals are fully occupied with d^{10} shell at high binding energy, similar to the situation in ThCr₂Si₂ structural ACu₂As₂ (A = Ca, Sr, Ba)³⁴. Just like the Fe-pnictide superconductors, the states around the E_F (from -2.0 to 2.0 eV) are mostly the Fe-3d states.

At the E_F , the DOS is $N(E_F)=3.3 \text{ eV}^{-1}$ per formulae. From $N(E_F)$, the calculated bare susceptibility and specific heat coefficient are $\chi_0=1.07 \times 10^{-4} \text{ emu/mol}$ and $\gamma_0=7.85 \text{ mJ}/(\text{K}^2 \cdot \text{mol})$, respectively. Our calculated specific heat coefficient is only $\frac{1}{5}$ as the experimental value $\gamma_0=40 \text{ mJ}/(\text{K}^2 \cdot \text{mol})$ ²⁹. Such high value may be due to nearness to a magnetic quantum critical point²⁹. In Figs.1(a) and 1(b), the Fe-3d contribution to $N(E_F)$ is more than 3 eV^{-1} per atom, which places the material near the Stoner itinerant magnetism due to the Stoner criterion³⁵: $N(E_F)I > 1$ (I is the Stoner parameter of Fe $I \sim 0.7-0.8$ ³⁶).

Comparing the DOS of CuFeSb [Fig. 1(b)] with that of CuFeAs, we find that the p-d hybridization between Sb-5p states and Fe-3d states is weaker than the hybridization between Fe-3d and As-4p. This enhances the itinerant character of CuFeSb. The larger Z_{Sb} may be responsible for such p-d hybridization reduction. Besides, it is interesting to note that the Fe bandwidth of CuFeSb is 0.3 eV narrower than that of CuFeAs, due to the longer Fe-Fe distance in the Sb compound (2.782 Å vs 2.648 Å). Such band narrowing may enhance the magnetic Fe moment in CuFeSb.

The projected band structure of CuFeAs is presented in Fig.2, where the symbol size corresponds to the projected weight of Bloch states onto the Fe (a) $d_{r^2-3z^2}$, (b) $d_{x^2-y^2}$, (c) d_{xy} , and (d) $d_{yz/zx}$ orbitals. There are four bands (two hole-like bands around the $\Gamma(0, 0, 0)$ point and two electron-like bands around the $M(\pi, \pi, 0)$) crossing the E_F , which is in consistency with the metallic resistance. The band dispersion along symmetry lines near the E_F quite resembles to that of LiFeAs and MgFeGe³⁷, where the former is a superconductor and the later is a ferromagnetic metal³⁸. The bands around E_F (from -1.0 to 1.0 eV) are mostly derived from d_{xy} and $d_{yz/zx}$ orbitals [Figs. 2(c) and 2(d)], while the states

TABLE I: Calculated total energies (with respect to the NM state), magnetic moments of Fe atoms, and DOS at E_F [$N(E_F)$] of CuFeAs and CuFeSb in the NM, FM, checkerboard, and stripe AF states respectively. The energy of NM state is set to zero.

	CuFeAs			CuFeSb		
Order	Energy (meV)	Moment (μ_B)	$N(E_F)$ (eV^{-1})	Energy (meV)	Moment (μ_B)	$N(E_F)$ (eV^{-1})
NM	0	0	3.3	0	0	3.97
FM	-213.21	2.27	2.91	-293.79	2.36	1.98
AF1	-84.09	1.86	4.18	-156.92	2.07	3.57
AF2	-151.85	1.84	3.48	-215.58	2.07	3.91

FIG. 2: (Color online) Projected band structure of CuFeAs in the NM configuration, where the symbol size corresponds to the projected weight of Bloch states onto the Fe (a) $d_{r^2-3z^2}$, (b) $d_{x^2-y^2}$, (c) d_{xy} , and (d) $d_{yz/zx}$ orbitals, with GGA formula. The four bands crossing the E_F are separately noted by the different colors.

FIG. 3: (Color online) Projected band structure of CuFeSb in the NM configuration, where the symbol size corresponds to the projected weight of Bloch states onto the Fe (a) $d_{r^2-3z^2}$, (b) $d_{x^2-y^2}$, (c) d_{xy} , and (d) $d_{yz/zx}$ orbitals, with GGA formula. The four bands crossing the E_F are separately noted by the different colors.

FIG. 4: (Color online) The Fermi surfaces of (a) CuFeAs and (b) CuFeSb, each band is shown separately .

of $d_{x^2-y^2}$ and $d_{r^2-3z^2}$ have very little contribution [Figs. 2(a) and 2(b)]. Such orbits character is similar to the conventional iron-based materials. The projected band structure of CuFeSb (Fig. 3) is similar to that of CuFeAs.

The FS topology is an important issue in the iron-based superconductors^{11,13-15}, so we present the FS of CuFeAs and CuFeSb in Figs 4(a) and 4(b), respectively. There are five FS sheets, originating from four bands across the E_F (Figs. 2 and 3). Their 2D character reflects the anisotropic electronic structure, in consistent with the anisotropic resistivity ($\rho_c/\rho_{ab} \approx 8.2$)²⁹. In combination with Fig. 2 (Fig. 3), the three-dimensional (3D) character plate-shaped sheet around Z-point is hole type and contributed by the mixture of three 3d orbitals ($d_{x^2-y^2}$, d_{zx} , and d_{yz}), red and green lines in Fig. 2 (Fig. 3). Along the Γ -Z line, there are two hole-like FS sheets. The small pocket shows strong 3D character, while the larger cylinder-shaped sheet shows very well 2D character. The small 3D pocket is primarily $d_{yz/zx}$ characteristic, while the 2D cylinder sheet mainly has d_{xy} character. Except for the above mentioned three hole-like FS sheets, two electron-like FS sheets exist at the Brillouin zone corner along M-A line and display a little dispersion along K_z . From Figs. 2(c) and 2(d) [Figs. 3(c) and 3(d)] we can see that these electron-like FS sheets have d_{xy} , d_{yz} , and d_{zx} character, which is similar to that of LiFeAs and MgFeGe³⁷.

In order to determine the true magnetic ground state of CuFeAs and CuFeSb, we studied four different magnetic phases and summarized the results in Table 1. For both compounds, the FM state is the most stable state, which is consistent with the experimental result of CuFeSb²⁹. For CuFeAs, our calculated results support Qian's conclusion (FM state)²⁹ rather than Thakur's report (AF state)²⁸. The calculated magnetic moments of Fe ions in CuFeAs and CuFeSb are comparable to the theoretical values of other iron based materials. For CuFeSb, the experimental moment is $1.70 \mu_B/\text{Fe}$ ³⁰, which is a little smaller than calculated result. However, the experiment Fe moment of nonstoichiometric $\text{Cu}_x\text{Fe}_{1+y}\text{As}$ is only $0.33 \mu_B/\text{Fe}$ ²⁹, which is rather smaller than the theoretical value. The Cu vacancies in $\text{Cu}_x\text{Fe}_{1+y}\text{As}$ might associate with the moment reduction²⁹.

Just like LaOFeAs ²¹, we map the total energies to the J_1 - J_2 Heisenberg model and deduce the nearest- and next-nearest-neighbor exchange coupling interactions as

$$J_1 = \frac{E_{FM} - E_{AF1}}{4S^2} \quad (1)$$

and

$$J_2 = \frac{E_{FM} + E_{AF1} - 2E_{AF2}}{8S^2}, \quad (2)$$

where E_{FM} , E_{AF1} , and E_{AF2} are the total energies of ferromagnetic, checkerboard, and stripe antiferromagnetic states and S is the Fe spin moment. For CuFeAs $J_1 = -32.28$ meV and $J_2 = 0.80$ meV, while $J_1 = -34.22$ meV and $J_2 = -2.44$ meV for CuFeSb. It is known that when $J_2 > |J_1|/2$, the system will give way to the stripe AF ground state¹⁸⁻²¹. Nevertheless, for CuFeAs and CuFeSb, the negative J_1 and relatively weak J_2 results in $J_2 \ll |J_1|/2$, which means that the FM state is more favorable. These exchange coupling interactions are consistent with the tendency towards ferromagnetism determined by the total energy calculation.

Fig.5 shows the DOS and projected DOS of CuFeAs [Fig.5(a) and 5(b)] and CuFeSb [Fig.5(c) and 5(d)] in the FM state, where their DOS are similar to each other. As illustrated in Fig.5, both Cu-3d states and As-4p (or Sb-5p) states distribute deeply below the E_F . Around the E_F , the states are mainly derived from the Fe-3d states, with up spin states being almost fully occupied and down spin states partially occupied. Compared with the NM state, the $N(E_F)$ of FM state substantially reduces, while the $N(E_F)$ of the AF states does not decrease. According to the Stoner mechanism³⁵, these compounds will favor the FM state, just like other itinerant magnetic systems YFe_2Ge_2 ³⁹ and CuFe_2Ge_2 ⁴⁰.

Previous studies indicate that the anion height (Z_{anion}) is important to determinate the electronic

TABLE II: Calculated the nearest- and next-nearest-neighbor exchange coupling interactions J_1 , J_2 , and $|J_1|/2$, versus Sb height.

Sb height (Å)	J_1 (meV)	J_2 (meV)	$ J_1 /2$ (meV)
1.64	2.38	12.65	1.19
1.69	-8.33	8.99	4.17
1.74	-18.34	5.16	9.17
1.79	-27.03	1.27	13.52
1.84	-34.22	-2.44	17.11
1.89	-40.43	-5.92	20.21

structure and even the magnetic ordering in the iron based materials^{25,27,41,42}. The large Z_{anion} is the remarkably character of CuFeAs and CuFeSb. To investigate the effect of Z_{anion} on magnetic ordering, we studied the stable energy and the Fe moment as a function of Z_{Sb} and presented the results in Fig.6. At the experimental height $Z_{Sb}=1.84$ Å, FM is the most stable state. When Z_{Sb} is decreased to 1.74 Å (experimental height Z_{As} of CuFeAs), the energy difference between FM and AF2 states reduces, although FM is still the most stable state. Further decreasing Z_{Sb} , the FM and AF2 states become degenerate at $Z_{Sb}=1.72$ Å, and finally the AF2 state becomes more stable than FM state for $Z_{Sb} < 1.72$ Å. The special value $Z_{Sb}=1.72$ Å is a Quantum Critical Point (QCP), where the compound translate from the FM state to stripe AF state. Such transition has also been predicated by Moon²⁷ in the FeTe compound. They found that FeTe switched its ground state from the stripe AF state to double-stripe AF state at $Z_{Te}=1.71$ Å²⁷. The Fe magnetic moment varying with Z_{Sb} is presented in Fig.6(b), which is in agreement with the magnetic moment dependence on the Z_{anion} of other iron-based superconductors. The Z_{anion} of LaOFeAs , BaFe_2As_2 , and FeTe are 1.31, 1.35, and 1.73 Å, respectively^{1,2,8}. At the same time, the Fe moments are $0.36 \mu_B$ for LaOFeAs ⁴³, $0.87 \mu_B$ for BaFe_2As_2 ⁴⁴, and $1.70 \mu_B$ for FeTe⁸.

To study how the Z_{Sb} influences on magnetic order, we map the total energies of different magnetic states to the J_1 - J_2 Heisenberg model and deduce the exchange coupling interactions J_1 and J_2 as a function of Z_{Sb} . In this model, the energy differences between various magnetic orderings are assumed predominantly by the contribution from the exchange interactions between the Fe moments with spin $\vec{S}$. So the Hamilton can be effectively modeled by the following the Heisenberg model:

$$H = J_1 \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j + J_2 \sum_{\langle\langle ij \rangle\rangle} \vec{S}_i \cdot \vec{S}_j \quad (3)$$

where $\langle ij \rangle$ and $\langle\langle ij \rangle\rangle$ denote the summation over the nearest- and next-nearest-neighbors, respectively. Though the contribution of itinerant electrons was

FIG. 5: (Color online) The DOS and projected DOS of (a, b) CuFeAs and (c, d) CuFeSb in the FM configure, with GGA formula.

FIG. 6: (Color online) (a) The relative total energy with respect to the FM ground state ($Z_{Sb}=1.84\text{\AA}$) and (b) the magnetic moment of Fe versus Sb height calculated for the FM, AF1, and AF2 phases.

missed in this model and our system was still away from the fully localized insulating region, previous study confirmed that it captured the substantial physics on the magnetic structures of iron based materials^{18–22}. The variations of J_1 and J_2 as a function of Z_{Sb} are summarized in Table 2. We find that the magnetic phase can be divided into two parts: 1. in the range $1.74\text{\AA} \leq Z_{Sb} \leq 1.89\text{\AA}$, where $J_1 < 0$ and $J_2 < |J_1|/2$, the compounds are in the FM state; 2. for $Z_{Sb} < 1.74\text{\AA}$, where $J_2 > |J_1|/2$, the stripe AF is the ground state. A similar FM-to-AF2 transition and J_1 - J_2 behavior were also found in CuFeAs, but the critical value is $Z_{As} = 1.66\text{\AA}$, smaller than $Z_{Sb} = 1.72\text{\AA}$ in CuFeSb and $Z_{Te} = 1.71\text{\AA}$ in FeTe²⁷. The small radius of As ion compared to Sb and Te ions might be the reason for the smaller critical value Z_{As} .

FIG. 7: (Color online) (a) Atomic structure of the FeSb layer, where Z_{Sb} is distance from Sb atom to the Fe atoms plane. (b) The dominant super-exchange actions are those between both a pair of nearest-neighbor (NN) Fe spins (J_1) and a pair of next-nearest-neighbor (NNN) Fe spins (J_2). The process contributing to the NNN super-exchange interaction between a pair of electrons. It involves the same 4p orbital, leading to an AF J_2 . The process contributing to (c) d-d NN interaction J_1 (FM) and (d) d-p-d NNN interaction J_2 (AF).

The reason why reducing $Z_{Sb(As)}$ will decrease the NN interaction J_1 but increase the NNN interaction J_2 can be understood by the schematic diagram of Fig.7. When the $Z_{Sb(As)}$ is shortened, the d-p-d NNN interaction J_2 (AF) will increase because that the $P_{x/y}$ -orbitals of Sb(As) atom come nearly to the Fe-atoms plane and then enhance the d-p-d exchange integral. But the

d-d NN interaction J_1 (FM) will be reduced when the Sb(As) atoms come nearly to the Fe-atoms plane. At some special $Z_{Sb(As)}$ value, i.e. the Quantum Critical Point (QCP), the compounds will translate from the FM state to stripe AF state.

IV. SUMMARY

In summary, by the first-principles calculations, we studied the electronic structures and magnetism of CuFeAs and CuFeSb. In the nonmagnetic state, their DOS, orbits character, band structure, and Fermi surface show similarities to those of other iron based superconductors. The total energy calculations indicate

that the ground state of these materials is the ferromagnetic state. Such ferromagnetic ground state is owing to the large anion height Z_{anion} , which reduces the d-P-d NNN interaction J_2 (AF) and increases d-d NN interaction J_1 (FM). The anion height Z_{anion} is the key tuning parameter for these two competing magnetic interactions (AF and FM), and it can switch the ground state from the AF state to FM state.

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