Evidence the ferromagnetic order on CoSb layer of LaCoSb

Muyuan Zou,1,∗ Jianan Chu,2,∗ Tianzhong Yuan,1 Xinyuan Wei,1 Peng Cheng,4 Da Jiang,5,6 Xuguang Xu,6 Zhenghua An,1,7 Gang Mu,6,1 and Wei Li1,7,3

1 State Key Laboratory of Surface Physics and Department of Physics, Fudan University, Shanghai 200433, China
2 State Key Laboratory of Functional Materials for Informatics, Shanghai Institute of Microsystem and Information Technology, Chinese Academy of Sciences, Shanghai 200050, China
3 University of Chinese Academy of Sciences, Beijing 100049, China
4 Department of Physics, Renmin University of China, Beijing 100872, China
5 Center of Materials Science and Optoelectronics Engineering, University of Chinese Academy of Sciences, Beijing 100049, China
6 School of Physical Science and Technology, ShanghaiTech University, Shanghai 201210, China
7 Collaborative Innovation Center of Advanced Microstructures, Nanjing 210093, China

(Dated: November 26, 2019)

The emergence of unconventional superconductivity is generally considered to be related with magnetic spin fluctuations. Unveiling the intriguing behaviours of magnetic spin fluctuations in mother compounds with layered transition metal ions may shed light on the search for exotic superconductors. Here, based on the framework of the first-principles calculations, we theoretically propose the LaCoSb2 as a candidate mother compound of cobalt-based superconductors, which is a weak antiferromagnetic layered metal but has an in-plane ferromagnetic order of 0.88 µB on Co sites. Importantly, this theoretical finding is supported by our magnetization measurements on polycrystalline samples of the LaCoSb2 experimentally. These results imply a possible p-wave superconductor hosted in the LaCoSb2, once the emergence of superconductivity locates in the vicinity of the verge of the ferromagnetic order, having potential applications in topological quantum computing in future.

Introduction.—The studies on the topological superconductors1–3 have triggered enormous research interests during the recent years, ascribing to these systems hosted the Majorana quasiparticles4 which obey non-Abelian statistics and can be used to encode and manipulate quantum information in a topologically protected manner. In solid state systems, the p-wave superconductors5 or ν = 5 2 fractional quantum Hall states6 are considered to exhibit Majorana quasiparticles. The first candidate chiral p-wave superconductor is Sr2RuO4 evidenced by previous NMR measurement,7 which breaks the time-reversal symmetry.8 However, a recent NMR measurement contradicts the previous finding attributing to the heat-up effect in Knight shift in the NMR experiment.9

Alternatively, a prominent theoretical study predicts the appearance of Majorana bound states at the interface between a topological insulator and a conventional superconductor10. A generic theory without any topological insulator is also proposed that considering the combination of Rashba spin-orbit coupling and Zeeman effect as well as the proximity effect from an s-wave superconductor in a two-dimensional metal will induce an effective p-wave superconductor11. Experimentally, the indictions of Majorana bound states have been reported in various systems, including the indium antimonide nanowires in contact with the superconducting12,13 at the edges of a chain of iron atoms formed on the surface of superconducting lead14, quantum spin liquid15, and a quantum anomalous Hall effect/superconductor hybrid device16, as well as iron-based superconductors17.

In this Letter, we theoretically propose the LaCoSb2 as a possible candidate topological superconductor that once the superconductivity locates in the vicinity of the verge of ferromagnetic (FM) order on CoSb layer. LaCoSb2 shown in Fig. 1(a) has a similar crystal structure to the 112-type iron-based superconductor.2,18–20 Similar to the electronic properties of layered iron-based superconductor,2–5,20 the conducting electrons mainly come from the contribution of Co 3d states partially hybridized with Sb 5p states on CoSb layer of LaCoSb2. Previous first-principles calculations demonstrate that the nonmagnetic (NM) state of LaCoSb2 displays a behavior of high-symmetry line semimetal.21 Surprisingly, the monolayer films of CoSb have been successfully grown on SrTiO3(001) substrates by molecular beam epitaxy, and observed symmetric superconducting gap around the Fermi level with coherence peaks at around ± 6 meV by in situ scanning tunneling spectroscopy,22 which is three times smaller compared with monolayer films of FeSe on SrTiO3(001) substrates.23 Furthermore, the ex situ magnetization measurements demonstrate the superconducting transition temperature of Tc ≈ 14 K for CoSb/SrTiO3. It is also worth pointing out that the presence of a weak net FM moment in CoSb/SrTiO3 has been observed in the magnetization as a function of magnetic field, although they explain the nature of FM contribution from the tellurium capping layer.24 Interestingly, our first-principles calculations find a weak antiferromagnetism but an in-plane FM order of 0.88 µB on Co sites to be the groundstate for LaCoSb2. Additionally, our magnetization measurements confirm the presence of antiferromagnetic (AFM) order in LaCoSb2 with the magnetic moment of 0.78 µB experimentally, in good...
agreement with the theoretical findings. Thus, LaCoSb$_2$ becomes a candidate mother compound of cobalt-based superconductors, when the charge carriers are gradually introducing into the mother compound, such as the hole-like carriers, the FM order is suppressed monotonously and the superconductivity emerges in the vicinity of the verge of the FM order, making the LaCoSb$_2$ to be a possible $p$-wave superconductor.

The First-Principles Calculations.—The calculations in this work are performed using the all-electron full potential linear augmented plane wave plus local orbitals (FP-LAPW+lo) method as implemented in the WIEN2k code. The exchange-correlation potential is calculated using the generalized gradient approximation as proposed by Perdew, Burke, and Ernzerhof. Since the spin-orbit coupling strength is proportional to $Z^4$ (where $Z$ is the atomic number; $Z = 51$ for Sb), the spin-orbit coupling is nonnegligible for the heavier atoms compound of the LaCoSb$_2$. Therefore, the spin-orbit coupling is included with the second variational method throughout the calculations. Furthermore, a 1000 $k$-point is chosen to ensure the calculation with an accuracy of 10$^{-5}$ eV, and all structures (lattice constants as well as internal coordinates) are performed using the values of experimental crystal structure shown in Fig. 1(a).

Firstly, we focus on the NM state behaviour of LaCoSb$_2$, which means no spin polarization is allowed on the Co ions in the calculations. Such a study can provide a reference for inspecting that the magnetization state is favorable. Fig. 1(b) shows the electronic energy band structure of NM state for LaCoSb$_2$, which has much more complicated electronic dispersive features than that for the 112-type iron-based superconductor. In contrast to the five bands across the Fermi level in iron-based superconductors, there are only three bands across the Fermi level for the cobalt-based material of LaCoSb$_2$. The Fermi surface topologies are shown in Fig. 1(d)-(f). Verifying the orbital characteristics of the energy bands at around the Fermi surface, we notice the prominent contributions stemming from the Co $d_{xy}$ and $d_{yz}$ orbitals. From the viewpoint of crystal field theory, the Co ions are coordinated by the Sb tetrahedron, and the crystal field will normally split the five Co 3$d$ orbitals into the low-lying twofold $e_g$ ($d_{xy}$ and $d_{xz}$) orbitals and up-lying threefold $t_{2g}$ ($d_{xz}$, $d_{yz}$, and $d_{z^2}$) orbitals opposite the octahedral case. However, when taking the Coulomb interaction into account, the actually instance by analyzing the orbital dependent energy band structure is opposite that we expect from a simple tetrahedra crystal field: the low-lying manifold is threefold ($t_{2g}$) and the up-lying manifold is twofold ($e_g$). For the Co$^{3+}$ ion, the nominal number of 3$d$ electrons is 6, the low-lying $d_{xz}$ and $d_{yz}$ orbitals are nearly fully occupied, and leave the $d_{xy}$ and $d_{z^2}$ orbitals to be partially occupied due to the strong Hund’s coupling effect. Since the atomic radii of Sb is much large, it drives the enhancement of the interlayer covalent bonds, as a result of the strong three dimensionality of Fermi surface topologies shown in Fig. 1(c) and (f). Additionally, it is interesting to point out that there is an electron-like pocket with nearly cylindrical shape located at around the $M$ point shown in Fig. 1(d), suggesting a strong two-dimensional behavior, similar to the electron pocket in 112-type iron-based superconductor. Furthermore, previous first-principles calculations have demonstrated that the band structure of NM state for LaCoSb$_2$ displays a behavior of high-symmetry line semimetal in consistent with our present calculations.

The calculated density of states (DOS) and the projected DOS (PDOS) on Co 3$d$ and Sb 5$p$ orbitals of LaCoSb$_2$ are shown in Fig. 1(c). It can be seen that
TABLE I. The calculated total energy of various magnetic ordering states of LaCoSb$_2$. $\Delta E$ is the total energy difference per Co atom referenced to the NM state, and $m_{Co}$ is the local magnetic moment on Co.

|                | FM  | AFM | A-AFM | c-AFM |
|----------------|-----|-----|-------|-------|
| $\Delta E$ (meV/Co) | -80.86 | -3.54 | -81.68 | -37.15 |
| $m_{Co}$ (\mu_B)  | 0.87 | 0.30 | 0.88  | 0.69  |

the conduction electrons mainly come from the contribution of Co 3$d$ states partially hybridized with Sb 5$p$ states. Verifying the value of DOS at the Fermi level, $N(E_f) = 2.28$ states per eV per Co atom, we notice that this value is much larger than that in the iron-based superconductors.\textsuperscript{20} According to the Stoner criterion\textsuperscript{20}, while magnetism may occur with lower values of the DOS, it must occur within a band picture if the Stoner criterion, $N(E_f) \times I > 1$, is met [the NM electronic structure becomes unstable against magnetic states in this case], where $I$ is the Stoner parameter, which takes values of 0.7 – 0.9 eV for ions near the middle of the 3$d$ series (note that the effective $I$ can be reduced by hybridization), suggesting the NM state is unstable against the magnetic states for LaCoSb$_2$.

To explore the groundstate with magnetic ordering of LaCoSb$_2$, we have calculated four different possible magnetic ordering states in the Co layer with FM, Néel-AFM, and A-type AFM (A-AFM)\textsuperscript{33} orders, as well as collinear AFM (c-AFM) order (align FM order along a direction and AFM order along the other direction in the Co-Co square lattice layer, similarly to that in LaOFeAs\textsuperscript{34,35,36}). The corresponding total energies of various magnetic ordering states are listed in Table I. It is shown that an A-AFM order with the FM ordered in Co layers and AFM ordered in between Co layers is the lowest energy state for LaCoSb$_2$. The calculated magnetic moment is 0.88 $\mu_B$ on Co atoms.

The calculated low energy band structure and the corresponding total DOS and the PDOS on one of the Co 3$d$ and Sb 5$p$ orbitals, as well as the orbital resolved PDOS on Co 3$d$ states, given the A-type AFM ordering state in LaCoSb$_2$ are shown clearly in Fig. 2. Compared with the NM state shown in Fig. 1, we find that most of the states around the Fermi level are gapped by the A-AFM order. The corresponding electronic DOS at the Fermi level is $N(E_f) = 0.45$ states per eV per Co atom, which is significantly less than that of the NM state (2.28 states per eV per Co atom), as is intuitively expected.

Furthermore, the calculated orbital dependent PDOS in Fig. 2(c) suggests the electrons with Co 3$d_{xy}$ and 3$d_{z^2}$ orbitals mainly contributing to the conducting electron. This result is also consistent with our aforementioned discussion within the framework of crystal field theory. Clarifying the role of the magnetic spin fluctuations may further provide an insight into concerning the mechanism of superconductivity that is possibly driven by electron-electron correlation.

In order to quantify the magnetic interactions for revealing microscopic spin fluctuation effects on LaCoSb$_2$, we consider a phenomenological theoretical Heisenberg model on the Co atoms as follows:\textsuperscript{37}

\[ \hat{H} = J_1 \sum_{\langle i, j \rangle} \vec{S}_i \cdot \vec{S}_j + J_2 \sum_{\langle \langle i, j \rangle \rangle} \vec{S}_i \cdot \vec{S}_j + J_\perp \sum_{\langle i, j \rangle} \vec{S}_i \times \vec{S}_j, \]

where $\vec{S}$ is the magnitude of Co spin. The $\langle i, j \rangle$ and $\langle \langle i, j \rangle \rangle$ denote the summation over the nearest neighbor and next-nearest neighbor sites, respectively. The parameters $J_1$ and $J_2$ describe the nearest neighboring and next-nearest neighboring intralayer exchange interactions, respectively, and $J_\perp$ denotes the nearest neighboring interlayer exchange interaction. From the calculated energy data for various magnetic configurations in Table I, the magnetic exchange couplings $J_1 = -19.33$ meV, $J_2 = -1.26$ meV, and $J_\perp = 0.41$ meV are found for LaCoSb$_2$, suggesting the FM order in the Co layer and the weak AFM order along the interlayer of Co. The strong FM order occurs in intralayer mainly originating from the superexchange interaction with strong Hund’s coupling mediated by Sb 5$p$ orbitals.\textsuperscript{38} Importantly, it is worth pointing out that the FM order on CoSb layer has also been observed by magnetization measurements in monolayer films of CoSb grown in SrTiO$_3$ substrates by molecular beam epitaxy, although they explain the nature of FM contribution from the tellurium capping layer.\textsuperscript{39} Furthermore, we also provide our experimental measurements in the following section to further solidify the theoretical prediction of the presence of the magnetic ordering in the bulk system of LaCoSb$_2$.

**Experimental measurements.**— We experimentally synthesized the LaCoSb$_2$ polycrystalline samples by an arc-melting method as described in the previous literature,\textsuperscript{21} whose the crystal structure is shown in Fig. 1(a), to verify the theoretical findings of the magnetic ordering in the bulk system of LaCoSb$_2$. In Fig. 3(a), we show the electric transport measurements on the LaCoSb$_2$ as a function of the temperature using the Physical Property Measurement System (PPMS DynaCool) made by Quantum Design. The electric resistivity decreases monotonously with cooling temperature, indicating a typical metallic behavior of LaCoSb$_2$. This experi-
ment system (Quantum Design MPMS3), which displays the temperature using the magnetic property measurement is in good agreement with our first-principles calculations shown in Fig. 3(b). Additionally, it is interesting to point out that the magnitude of electric resistivity is about 1-2 orders lower than the iron-based superconductors. Furthermore, we also measure the magnetic susceptibility of the LaCoSb$_2$ as a function of the temperature using the magnetic property measurement system (Quantum Design MPMS3), which displays a monotonous increase with cooling temperature, shown in Fig. 3(b). This behavior is fitted by a generalized Curie-Weiss law

\[ \chi(T) = \chi_0 + \frac{C}{T - \theta}, \]  

(2)

where \( \chi_0 \) is a positive constant corresponding to the temperature-independent Pauli contribution of the electron gas. The fitting curve is given in Fig. 3(b) as shown by the red solid line, indicating a good quality of Curie-Weiss fitting. Through the Curie-Weiss fitting, the obtained \( \theta \) value is -2.9 K. The negative value of \( \theta \) suggests an AFM coupling in LaCoSb$_2$. From the fitting value of \( C = 382 \text{ emu} \cdot \text{K/mol} \), we derive the effective magnetic moments \( \mu_{eff} = 0.78 \mu_B \) on Co sites of LaCoSb$_2$, which is consistent with the theoretical prediction qualitatively, but has a bit smaller value than the theoretical one (0.88\( \mu_B \)) in quantity. This is because that the difference between the theoretical and experimental finding may originate from the the polycrystalline sample of LaCoSb$_2$ in experiments. Therefore, these experimental findings further solidify the theoretical prediction of the weak AFM ordering in interlayers and FM ordering within each layers in LaCoSb$_2$.

**Conclusion.**—Using the first-principles calculations, we systematically study the electronic and magnetic structures of LaCoSb$_2$ in theory, and propose a weak AFM ordering metal with the FM order in CoSb layers for the LaCoSb$_2$. This theoretical finding is further supported by our magnetization measurements on the synthesized polycrystalline samples of the LaCoSb$_2$ in experiments. These results suggest the LaCoSb$_2$ as a possible candidate mother compound of cobalt-based superconductors, once the FM order suppresses and the superconductivity emerges as gradually introducing the charge carriers into the systems, such as the hole-like carriers. Since the emergence of the superconductivity locates in the vicinity of the verge of the FM order, it makes the doped LaCoSb$_2$ to be a possible \( p \)-wave superconductor having the potential applications in topological quantum computing in future.

This work was supported by the National Natural Science Foundation of China (Grant No. 11927807) and the Natural Science Foundation of Shanghai of China (Grants No. 18JC1420402 and No. 19ZR1402600). W. L. also acknowledges the start-up funding from Fudan University.

* M.Y. Zou and J.N. Chu contributed equally to this work.

† E-mail: mugang@mail.sim.ac.cn

‡ E-mail: w_li@fudan.edu.cn

1 X.-L. Qi and S.-C. Zhang, *Topological insulators and superconductors*, Rev. Mod. Phys. 83, 1057 (2011).
2 C. W. J. Beenakker, *Search for Majorana Fermions in Superconductors*, Annu. Rev. Condens. Matter Phys. 4, 113 (2013).
3 M. Sato and Y. Ando, *Topological superconductors: a review*, Rep. Prog. Phys. 80, 076501 (2017).
4 S. R. Elliott and M. Franz, *Majorana fermions in nuclear, particle, and solid-state physics*, Rev. Mod. Phys. 87, 137 (2015).
5 C. Nayak, S. H. Simon, A. Stern, M. Freedman, and S. Das Sarma, *Non-Abelian anyons and topological quantum computation*, Rev. Mod. Phys. 80, 1083 (2008).
6 D. A. Ivanov, *Non-Abelian Statistics of Half-Quantum Vortices in p-Wave Superconductors*, Phys. Rev. Lett. 86, 268 (2001).
7 N. Read and D. Green, *Paired states of fermions in two dimensions with breaking of parity and time-reversal symmetries and the fractional quantum Hall effect*, Phys. Rev. B 61, 10267 (2000).
8 Y. Maeno, H. Hashimoto, K. Yoshida, S. Nishizaki, T. Fujita, J. G. Bednorz, and F. Lichtenberg, *Superconductivity*...
in a layered perovskite without copper, Nature 372, 532 (1994).

K. Ishida, H. Mukuda, Y. Kitaoaka, K. Asayama, Z. Q. Mao, Y. Mori, and Y. Maeno, Spin-triplet superconductivity in \( \text{Sr}_2\text{RuO}_4 \) identified by \( ^{17} \text{O} \) Knight shift, Nature 396, 658 (1998).

A. Kapitulnik, J. Xia, E. Schemm, and A. Palevski, Polar Kerr effect as probe for time-reversal symmetry breaking in unconventional superconductors, New Journal of Physics 11, 055060 (2009).

A. Pustogow, Y. Luo, A. Chronister, Y.-S. Su, D. Sokolov, F. Jerzembeck, A. P. Mackenzie, C. W. Hicks, N. Kikutaga, S. Raghu, E. D. Bauer, and S. E. Brown, Pronounced drop of \( ^{17} \text{O} \) NMR Knight shift in superconducting state of \( \text{Sr}_2\text{RuO}_4 \), arXiv: 1904.00047 (2019).

K. Ishida, M. Manago, and Y. Maeno, Reduction of the \( ^{17} \text{O} \) Knight shift in the Superconducting State and the Heat-up Effect by NMR Pulses on \( \text{Sr}_2\text{RuO}_4 \), arXiv: 1907.12236 (2019).

L. Fu and C. L. Kane, Superconducting Proximity Effect and Majorana Fermions at the Surface of a Topological Insulator, Phys. Rev. Lett. 100, 096407 (2008).

J. D. Sau, R. M. Lutchyn, S. T. W. Tewari, and S. Das Sarma, Generic New Platform for Topological Quantum Computation Using Semiconducting Heterostructures, Phys. Rev. Lett. 104, 040502 (2010).

V. Mourik, K. Zuo, S. M. Frolov, S. R. Plissard, E. P. A. M. Bakkers, and L. P. Kouwenhoven, Signatures of Majorana Fermions in Hybrid Superconductor–Semiconductor Nanowire Devices, Science 336, 1003 (2012).

M. T. Deng, S. Vaitiekūnas, E. B. Hansen, J. Danon, M. Leijnse, K. Flensberg, J. Nygård, P. Kroegstrup, and C. M. Marcus, Majorca bound state in a coupled quantum-dot hybrid-nanowire system, Science 354, 1557 (2016).

S. Nadj-Perge, I. K. Drozlov, J. Li, H. Chen, S. Jeon, J. Seo, A. H. MacDonald, B. A. Bernevig, and A. Yazdani, Observation of Majorana fermions in ferromagnetic atomic chains on a superconductor, Science 346, 602 (2014).

A. Banerjee, C. A. Bridges, J.-Q. Yan, A. A. Aczel, L. Li, M. B. Stone, G. E. Granroth, M. D. Lumsden, Y. Yu, J. Knolle, S. Bhattacharjee, D. L. Kovrizhin, R. Moessner, D. A. Tennant, D. G. Mandrus, and S. E. Nagler, Proximate Kitaev quantum spin liquid behaviour in a honeycomb magnet, Nature Materials 15, 733 (2016).

Q.-L. He, L. Pan, A. L. Stern, E. C. Burks, X. Che, G. Yin, J. Wang, B. Lian, Q. Zhou, E.-S. Choi, K. Murata, X. Kou, Z. Chen, T. Nie, Q. Shao, Y. Fan, S.-C. Zhang, K. Liu, J. Xia, and K.-L. Wang, Chiral Majorca fermion modes in a quantum anomalous Hall insulator–superconductor structure, Science 357, 294 (2017).

D. Wang, L. Kong, P. Fan, H. Chen, S. Zhu, W. Liu, L. Cao, Y. Sun, S. Du, J. Schneeloch, R. Zhong, G. Gu, L. Fu, H. Ding, and H.-J. Gao, Evidence for Majorana bound states in an iron-based superconductor, Science 352, 333 (2018).

A. Leithe-Jasper and P. Rogl, The crystal structure of \( \text{NdFe}_1-x\text{Sr}_x \text{Sb}_2 \) and isotopic compounds \( \text{RE(Fe, Ce, Pr, Sm, Gd)}_2 \text{Sb}_2 \) \( (\text{RE=La, Ce, Pr, Sm, Gd}) \), Journal of Alloys and Compounds 203, 133 (1994).

N. Katayama, K. Kudo, S. Onari, T. Mizukami, K. Sugawara, Y. Sugiyama, Y. Kitahama, K. Iba, K. Fujimura, N. Nishimoto, M. Nohara, and H. Sawa, Superconductivity in \( \text{Ca}_{1-x}\text{La}_x\text{FeAs}_2 \): A Novel 112-Type Iron Pnictide with Arsenic Zigzag Bonds, J. Phys. Soc. Jpn. 82, 123702 (2013).

H. Yakita, H. Ogin, T. Okada, A. Yamamoto, K. Kishio, T. Tohei, Y. Ikhara, Y. Gotoh, H. Fujisahi, K. Kataoka, H. Eisaki, and J.-i. Shimoyama, A New Layered Iron Arsenide Superconductor: \((\text{Ca,Pr})\text{FeAs}_2\), J. Am. Chem. Soc. 136, 846 (2014).

W. Li, S. Dong, C. Fang, and J. Hu, Block antiferromagnetism and checkerboard charge ordering in the alkali-doped iron selenides \( \text{R}_{1-x}\text{Fe}_2\text{As}_2 \), Phys. Rev. B 85, 100407(R) (2012).

W. Li, J.-X. Zhu, Y. Chen, and C. S. Ting, First-principles calculations of the electronic structure of iron-pnictide \( \text{EuFe}_2(\text{As,P})_2 \) superconductors: Evidence for antiferromagnetic spin order, Phys. Rev. B 86, 155119 (2012).

T. Zhang, Y. Jiang, Z. Song, H. Huang, Y. He, Z. Fang, H. Weng, and C. Fang, Catalogue of topological electronic materials, Nature 566, 475 (2019).

C. Ding, G. Gong, Y. Liu, F. Zheng, Z. Zhang, H. Yang, Z. Li, Y. Xing, J. Ge, K. He, W. Li, P. Zhang, J. Wang, L. Wang, and Q.-K. Xue, Signature of Superconductivity in Orthorhombic CoSb Monolayer Films on \( \text{SrTiO}_3(001) \), ACS Nano 13, 10434 (2019).

Q.-Y. Wang, Z. Li, W.-H. Zhang, Z.-C. Zhang, J.-S. Zhang, W. Li, H. Ding, Y.-B. Ou, P. Deng, K. Chang, J. Wen, C.-L. Song, K. He, J.-F. Jia, S.-H. Ji, Y.-Y. Wang, L.-L. Wang, X. Chen, X.-C. Ma, and Q.-K. Xue, Interface-induced high-temperature superconductivity in single unit-cell FeSe films on \( \text{SrTiO}_3 \), Chin. Phys. Lett. 29, 037402 (2012).

D. J. Singh and L. Nordstrom, Planewaves, Pseudopotentials, and the LAPW Method, 2nd ed. (Springer-Verlag, Berlin, 2006), pp. 1C134.

P. Blaha, K. Schwarz, G. Madsen, D. Kvasnicka, and J. Luitz, in WIEN2K, An Augmented PlaneWave + Local Orbitals Program for Calculating Crystal Properties, edited by K. Schwarz (Technical Univesity Wien, Austria, 2001).

J. P. Perdew, K. Burke, and M. Erzerhof, Generalized gradient approximation made simple, Phys. Rev. Lett. 77, 3865 (1996).

W. Li, X.-Y. Wei, J.-X. Zhu, C. S. Ting, and Y. Chen, Pressure-induced topological quantum phase transition in \( \text{Sb}_2\text{Se}_3 \), Phys. Rev. B 89, 035101 (2014).

D. J. Singh, Electronic structure and doping in \( \text{BaFe}_2\text{As}_2 \) and \( \text{LiFeAs} \): Density functional calculations, Phys. Rev. B 78, 094511 (2008).

E. O. Wollan and W. C. Koehler, Neutron diffraction study of the magnetic properties of the series of perovskite-type compounds \( ([1-x]\text{La, xCa})\text{MnO}_3 \), Phys. Rev. 100, 545 (1955).

J. Dong, H. J. Zhang, G. Xu, Z. Li, G. Li, W. Z. Hu, D. Wu, G. F. Chen, X. Dai, J. L. Luo, Z. Fang, and N. L. Wang, Competing orders and spin-density-wave instability in \( \text{La(0.1-x)}\text{Fe}_x\text{F}_4 \text{FeAs} \), Europhys. Lett. 83, 27006 (2008).

C. de la Cruz, Q. Huang, J. W. Lynn, J. Li, W. Ratcliff II, J. L. Zarestky, H. A. Mook, G. F. Chen, J. L. Luo, N. L. Wang, and P. Dai, Magnetic order close to superconductivity in the iron-based layered \( \text{LaO}_{1-x}\text{Fe}_x\text{FeAs} \) systems, Nature 453, 899 (2008).

Z. Zhou, W. T. Jin, W. Li, S. Nandi, B. Ouladdiaf, Z. Yan, X. Wei, X. Xu, W. H. Jiao, N. Qureshi, Y. Xiao, Y. Su, G. H. Cao, and Th. Brückel, Universal critical behavior in the fermionic superconductor \((\text{Eu}(\text{Fe}_{0.72}\text{Ru}_{0.28})_{2}\text{As}_2 \text{Fe}) \), Phys. Rev. B 100, 060406(R) (2019).
38 S. Maekawa, T. Tohyama, S. E. Barnes, S. Ishihara, W. Koshibae, and G. Khaliullin, *Physics of Transition Metal Oxides*, (Springer-Verlag Berlin Heidelberg GmbH, 2004).
39 G. Mu, B. Zeng, X. Zhu, F. Han, P. Cheng, B. Shen, and H. H. Wen, *Synthesis, structural, and transport properties of the hole-doped superconductor Pr$_{1-x}$Sr$_x$FeAsO*, Phys. Rev. B 79, 104501 (2009).
40 P. Amornpitoksuk, D. Ravot, A. Mauger, and J. C. Tedenac, *Structural and magnetic properties of the ternary solid solution between CoSb and Fe$_{1+\delta}$Sb*, Phys. Rev. B 77, 144405 (2008).