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Article

Keywords: monolayered CoSb superconductor, Non-unitary superconductivity, superconductivity, ferromagnetism

Posted Date: September 28th, 2020

DOI: <https://doi.org/10.21203/rs.3.rs-77943/v1>

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Non-unitary superconductivity in the monolayer of orthorhombic CoSb

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(Dated: September 12, 2020)

Abstract

Ferromagnetism and superconductivity are generally considered to be antagonistic phenomena in condensed matter physics. Here, we theoretically study the interplay between the ferromagnetic and superconducting orders in a recent discovered monolayered CoSb superconductor with an orthorhombic symmetry and net magnetization, and demonstrate the pairing symmetry of CoSb as a candidate of non-unitary superconductor with time-reversal symmetry breaking. By performing the group theory analysis and the first-principles calculations, the superconducting order parameter is suggested to be a triplet pairing with the irreducible representation of ${}^3B_{2u}$, which displays intriguing nodal points and non-zero periodic modulation of Cooper pair spin polarization on the Fermi surface topologies. These findings not only provide a significant theoretical insight into the coexistence of superconductivity and ferromagnetism, but also reveal the enhancement of exotic spin polarized Cooper pairing by ferromagnetic spin fluctuations in a triplet superconductor.

The search for exotic unconventional pairing superconductivity with time-reversal symmetry breaking is a fundamental issue in condensed matter physics. Among of them, the prominent chiral pairing superconductors originated from the contribution of orbital angular momentum of Cooper paired electrons, such as the chiral p -wave pairing topological superconductors^{1,2}, have received great attentions as they host the Majorana quasiparticles at the boundaries³⁻⁸, which is equivalent to the non-Abelian Moore-Read (Pfaffian) spin-triplet paired state in the fractional quantum Hall effect with filling factor of $5/2$ ⁹⁻¹¹, and has potential applications in the topological quantum computing¹²⁻¹⁷. Experimentally, the evidences of observing Majorana bound states have been extensively reported in various quantum systems, including the one-dimensional nanowires in contact with superconductors¹⁸⁻²², at the edges of iron-atoms chains formed on the surface of superconducting lead²³, at the interface between a topological insulator and an s -wave superconductor^{24,25}, and the quantum spin liquids²⁶, as well as the iron-based superconductors²⁷⁻³³.

Additionally, another class of superconductors with time-reversal symmetry breaking, the intriguing non-unitary pairing superconductors³⁴, originated from the contribution of spin angular momentum of Cooper paired electrons, are inspiring enormous research interests in the condensed matter communities recently. The richness of existing Majorana quasiparticles in three-dimensional high-symmetry non-unitary pairing superconductors has been theoretically proposed³⁵. So far, however, the only experimentally established non-unitary pairing is in the A_1 phase of superfluid ^3He in an applied high magnetic field³⁶⁻³⁸, although non-unitary paired states have been extensively reported in the heavy fermion superconductor UPt_3 related to the B phase at low temperature in an applied magnetic field³⁹⁻⁴², and in the noncentrosymmetric LaNiC_2 ^{43,44} and centrosymmetric LaNiGa_2 superconductors^{45,46} with the absence of an applied magnetic field.

In this paper, we theoretically propose the monolayered orthorhombic CoSb as a candidate of non-unitary pairing superconductor, which has been successfully grown on the $\text{SrTiO}_3(001)$ substrate by molecular beam epitaxy. Experimentally, symmetric superconducting gap around the Fermi level with coherence peaks at around ± 6 meV was observed by *in-situ* scanning tunneling spectroscopy (STS), accompanied with a weak net ferromagnetic (FM) moment lying in the basal plane found by *ex-situ* magnetization measurements⁴⁷. The pairing symmetry of this system, however, remains elusive in experiments. Theoretically, the group symmetry analysis suggests the pairing symmetry of monolayered CoSb to be a non-

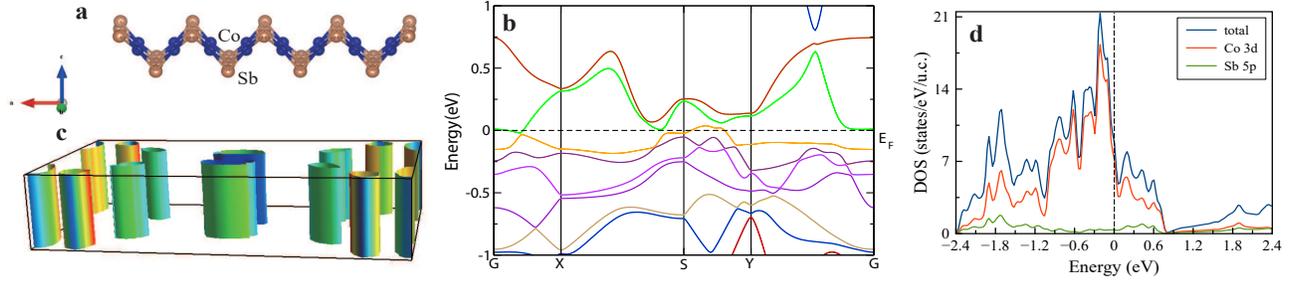


FIG. 1. The crystal structure and electronic structure of monolayered CoSb. (a) The schematic illustration of the crystal structure of monolayered orthorhombic CoSb. (b) The electronic band structure and (c) the corresponding Fermi surface topologies for the NM state of monolayered CoSb. (d) The total DOS and PDOS on Co $3d$ and Sb $5p$ orbitals for the NM state of monolayered CoSb. The Fermi energies are set to zero.

unitary triplet gap function of ${}^3B_{2u}$ or ${}^3B_{3u}$ symmetry with nodes. Within the framework of density-functional theory, the calculations demonstrate the ground state of monolayered CoSb to be a half metal with the easy axis of FM magnetization along the \hat{y} axis lying in the basal plane, which is consistent with experimental observation⁴⁷ and supports the group theory analysis that only spin-down electrons are responsible for the Cooper pairing in the non-unitary superconducting state. In the strong-coupling approximation, the superconducting order parameter in the monolayered CoSb is led to be a triplet pairing with the irreducible representation of ${}^3B_{2u}$, displaying intriguing nodal points and non-zero periodic modulation of Cooper pair spin polarization on the Fermi surface topologies. These findings imply the coexistence of ferromagnetism and superconductivity and the enhancement of exotic spin polarized Cooper pairing by FM spin fluctuations in the superconductor CoSb.

Results

Group symmetry analysis. Considering the D_{2h} point group of the superconducting orthorhombic CoSb monolayer shown in Fig. 1(a) with the time-reversal symmetry breaking⁴⁷, the superconducting pairing gap function $\Delta(\vec{k})$ can be factored into the basis functions with the irreducible representation of the group $SO(3) \times D_{2h}$ in the weak spin-orbit coupling limit^{48–50}, where \times and $SO(3)$ represent the direct product and all spin rotations, respectively. Similar to that in the centrosymmetric superconductor LaNiGa_2 ⁴⁵, this product group has a total of eight irreducible representations listed in Table I, including four one-dimensional

TABLE I. The upper and lower tables show the gap functions of the homogeneous superconducting states allowed by symmetry for a weak and a strong spin-orbit coupling, respectively. We have used the standard notation³⁴ $\hat{\Delta}(\vec{k}) = \Delta(\vec{k})i\hat{\sigma}_y$ for singlet states and $\hat{\Delta}(\vec{k}) = i[\mathbf{d}(\vec{k}) \cdot \hat{\sigma}]\hat{\sigma}_y$ for triplets, where $\hat{\sigma}$ is the vector of Pauli matrices, and \vec{k} is the momentum.

$SO(3) \times D_{2h}$	unitary state	non-unitary state
${}^1A_{1g}$	$\Delta(\vec{k}) = 1$	0
${}^1B_{1g}$	$\Delta(\vec{k}) = k_x k_y$	0
${}^1B_{2g}$	$\Delta(\vec{k}) = k_x k_z$	0
${}^1B_{3g}$	$\Delta(\vec{k}) = k_y k_z$	0
${}^3A_{1u}$	$d(\vec{k}) = (0, 0, 1)k_x k_y k_z$	$d(\vec{k}) = (1, -i, 0)k_x k_y k_z$
${}^3B_{1u}$	$d(\vec{k}) = (0, 0, 1)k_z$	$d(\vec{k}) = (1, -i, 0)k_z$
${}^3B_{2u}$	$d(\vec{k}) = (0, 0, 1)k_y$	$d(\vec{k}) = (1, -i, 0)k_y$
${}^3B_{3u}$	$d(\vec{k}) = (0, 0, 1)k_x$	$d(\vec{k}) = (1, -i, 0)k_x$

D_{2h}	Gap functions with strong spin-orbit coupling
A_{1u}	$d(\vec{k}) = (Ak_x, Bk_y, Ck_z)$
B_{1u}	$d(\vec{k}) = (Ak_y, Bk_x, Ck_x k_y k_z)$
B_{2u}	$d(\vec{k}) = (Ak_z, Bk_x k_y k_z, Ck_x)$
B_{3u}	$d(\vec{k}) = (Ak_x k_y k_z, Bk_z, Ck_y)$

singlet representations and four three-dimensional triplet representations. The latter have a gap function that transforms like a vector under spin rotations, resulting in the two possible ground states in a general Ginzburg-Landau theory⁴⁸. This leads to twelve possible gap functions listed in Table I, of which eight are unitary and four are non-unitary. Only the four non-unitary gap functions are non-trivially complex that can break the time-reversal symmetry. Furthermore, in accordance with the two-dimensionality of monolayered CoSb, we further eliminate the two states showing strong k_z dependence of the gap function. In contrast, there are only four possible gap functions and none of them could break time-reversal symmetry in the strong spin-orbit coupling limit, as listed in Table I. Therefore, from the viewpoint of symmetry, the superconducting orthorhombic CoSb monolayer has to be a non-unitary triplet pairing superconductor with a weak spin-orbit coupling, so that

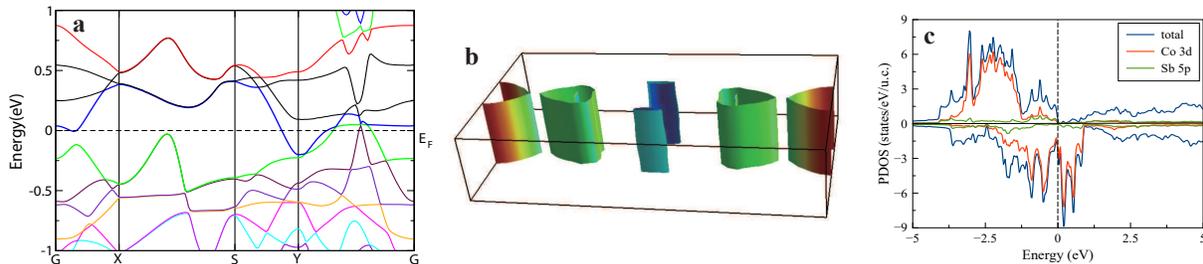


FIG. 2. The magnetic structure of monolayered CoSb. (a) The electronic band structure and (b) the corresponding Fermi surface topologies for the FM state of monolayered CoSb. (d) The PDOS on the spin-up and spin-down species of total, Co $3d$, and Sb $5p$ orbitals for the FM state of monolayered CoSb. The Fermi energies are set to zero.

the possible gap functions with ${}^3B_{2u}$ and ${}^3B_{3u}$ symmetry are only compatible with the experimental observation of time-reversal symmetry breaking⁴⁷. In them, only spin-down electrons participate in pairing, and thus there is an ungapped Fermi surface coexisting with another one with nodes (${}^3B_{2u}$ or ${}^3B_{3u}$).

The First-Principles Calculations. Figs. 1(b)-(d) show the non-magnetic (NM) electronic structures of monolayered orthorhombic CoSb, where no spin polarization is allowed on the Co ions. Such a study can provide a benchmark for inspecting whether the magnetically ordered state is favorable. From the calculated energy band structure and the corresponding Fermi surface topologies shown in Figs. 1(b) and (c), there are mainly two bands crossing the Fermi level contributing to the electron conduction in orthorhombic CoSb, in contrast to the four bands across the Fermi level in the tetragonal CoSb^{51,52}. Verifying the orbital characters of the energy bands around the Fermi level [see Fig. S1 in the supplementary information (SI) for details], we notice that the five Co $3d$ orbitals participate the electron conduction, implying the strong Hund's coupling in the Co $3d$ orbitals.

The calculated density of states (DOS) and the projected DOS (PDOS) on Co $3d$ and Sb $5p$ orbitals for the NM state of monolayered orthorhombic CoSb are shown in Fig. 1(d). It can be seen that the conduction electrons mainly come from the contribution of Co $3d$ states partially hybridized with mediated Sb $5p$ states. Inspecting the value of DOS at the Fermi level, $N(E_f) = 3.58$ states per eV per Co atom, we notice that this value is much larger than that in the tetragonal CoSb^{51,52} and the iron-based superconductors⁵³. While

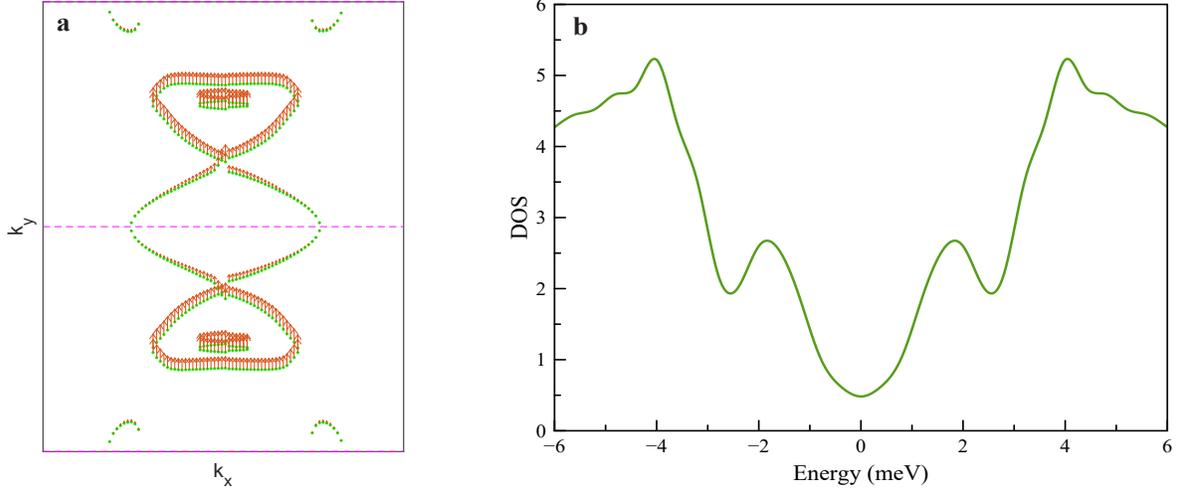


FIG. 3. The superconducting properties of monolayered CoSb. (a) A schematic plot for the gap nodal structure of non-unitary pairing on the Fermi surface topologies. The green dotted lines denote the Fermi surface topology of monolayered CoSb, and the magenta dashed lines denote the zero gap value of the order parameter $d(\vec{k}) = (1, -i, 0) \sin(k_y a_2)$ with the irreducible representation of ${}^3B_{2u}$. The vector plot of Cooper pair spin polarization $\langle \hat{S}_{\vec{k}} \rangle$ is also shown on the counters of Fermi surface topologies. (b) The DOS as a function of energy for the non-unitary superconducting state. The parameter of pairing amplitude is set as $\Delta_0 = 5$ meV.

magnetism may occur with lower values of the DOS, it must occur within a band picture if the Stoner criterion^{53,54}, $N(E_f) \times I > 1$, is met, where I is the Stoner parameter, taking values of 0.7 – 0.9 eV for ions near the middle of the 3d series (note that the effective I can be reduced by hybridization)⁵⁴, implying the NM state is unstable against the magnetic states for monolayered CoSb.

In order to capture the magnetic behavior of Co 3d states in the monolayered orthorhombic CoSb, we consider a two-dimensional phenomenologically theoretical Heisenberg model on the Co ion sites as follow^{52,53}:

$$\hat{H} = J_{1x} \sum_i \vec{S}_i \vec{S}_{i+\hat{x}} + J_{1y} \sum_i \vec{S}_i \vec{S}_{i+\hat{y}} + J_2 \sum_{\langle\langle i,j \rangle\rangle} \vec{S}_i \vec{S}_j, \quad (1)$$

where \vec{S} is the magnitude of Co spin. The $\langle\langle i,j \rangle\rangle$ denotes the summation over the next-nearest neighbor Co ion sites. The parameters J_{1x} and J_{1y} describe the nearest neighboring exchange interactions along the \hat{x} and \hat{y} direction shown in Fig. 1(a) with the labels of a and b , respectively, and J_2 denotes the next-nearest neighboring exchange interaction. From the

calculated energies for various magnetic configurations⁵⁵ (see SI in details), the magnetic exchange couplings $J_{1x} = 1.05$ meV, $J_{1y} = -46.46$ meV, and $J_2 = -2.98$ meV are found for the monolayered orthorhombic CoSb. The strong FM superexchange coupling strength along the \hat{y} axis could be understood through the Goodenough-Kanamori orthogonal rule^{56,57} at first glance that the interacting cations of Co atoms connected to the intervening anions of Sb form an angle of 74.1° ($\sim 90^\circ$), which promotes the mediated Sb $5p$ orbitals to be orthogonal to the two nearest neighboring Co $3d$ orbitals. Considering the strong Hund's coupling on Co $3d$ orbitals, the Co^{3+} ion with $3d^6$ electronic configuration favors the unpaired spin on Sb $5p$ orbitals to be parallelly aligned to the spin of the Co $3d$ orbitals, resulting in the FM exchange coupling. However, when the distance of 3.24 \AA ($= a_2$) between two nearest Co ion sites along \hat{y} axis is changed to 2.96 \AA ($= a_1/2$) along the \hat{x} axis and the bond angle of Co-Sb-Co is changed to 66.8° , the orthogonality between the Sb $5p$ and the two nearest neighboring Co $3d$ orbitals is weakened significantly and thus the antiferromagnetic superexchange coupling could be gradually emerged along the \hat{x} direction. Due to the strong FM exchange couplings on the CoSb layer, it suggests the ground state of CoSb to be a FM order⁵⁸, which is consistent with the magnetization measurements on the monolayered films of orthorhombic CoSb⁴⁷. Furthermore, the strong anisotropic FM superexchange interaction along the \hat{y} axis drives the easy axis of magnetization of CoSb towards the \hat{y} axis lying in the basal plane, which is also confirmed by the total energy calculations. The magnetic momentum of $1.83 \mu_B$ on Co ion sites are found (see details in Tables S1 & S2 in SI).

The calculated low-energy band structure, the corresponding Fermi surface topologies, and the PDOS on the spin-up and spin-down species of total, Co $3d$ and Sb $5p$ orbitals for the FM ordered state with fixed magnetization along the \hat{y} axis in the monolayered orthorhombic CoSb are shown in Fig. 2. Compared with the NM state shown in Fig. 1, we find that most of the bands around the Fermi level are gapped by the FM order. The corresponding electronic DOS at the Fermi level is $N(E_f) = 0.12$ and $N(E_f) = 1.48$ states per eV per Co atom for spin-up and spin-down species, respectively, which is significantly less than that of the NM state (3.58 states per eV per Co atom), demonstrating a half metal nature of the monolayered orthorhombic CoSb that the spin-up orbitals are fully occupied while the spin-down orbitals are partially occupied (see details in Figs. S2 & S3 in SI). This finding is consistent with the group theory analysis that only spin-down electrons are responsible for the Cooper pairs in the non-unitary superconducting state.

Theoretical Model Calculations. A simplified theoretical model of low-energy excitations in the non-unitary superconducting state is provided for further understanding of the behaviors of superconducting electrons based on the following BdG Hamiltonian:

$$\hat{H}_{sc} = \begin{pmatrix} \hat{H}_0(\vec{k}) & \hat{\Delta}_0(\vec{k}) \\ \hat{\Delta}_0^\dagger(\vec{k}) & -\hat{H}_0(\vec{k}) \end{pmatrix}, \quad (2)$$

where \vec{k} is the momentum of the excitation, $\hat{H}_0(\vec{k})$ describes an effective spin-dependent four-band normal-state free electron Hamiltonian obtained through an interpolation method by projecting the first-principles calculated bands shown in Fig. 2 onto the lowest two spin-dependent bands around the Fermi level^{59,60} in the momentum space, and $\hat{\Delta}_0(\vec{k}) = \Delta_0 \hat{\Delta}(\vec{k}) \otimes i\tau_y$ represents the pairing potential with a pairing amplitude of Δ_0 . In the tensor products, the first sector represents the spin channels $\sigma = \uparrow, \downarrow$ shown in the caption of Table I while the second represents the two band channels⁴⁶. Following the group symmetry analysis, the $\mathbf{d}(\vec{k})$ vector has two possible choices of $d(\vec{k}) = (1, -i, 0) \sin(k_y a_2)$ and $d(\vec{k}) = (1, -i, 0) \sin(k_x a_1)$, as listed in the Table I, corresponding to the irreducible representations of ${}^3B_{2u}$ and ${}^3B_{3u}$, respectively. Here we have assumed that the Cooper pairs carry the spin magnetization with the value of $\langle \hat{S}_{\vec{k}} \rangle = i\mathbf{d} \times \mathbf{d}^*$ ³⁴ along the \hat{y} axis in accordance with the FM magnetization obtained by the first-principles calculations. Since the pairing amplitude of Δ_0 is proportional to FM superexchange coupling strength within strong-coupling approximation, the triplet pairing state with the irreducible representations of ${}^3B_{3u}$ is energetically unfavorable rather than that of ${}^3B_{2u}$, to avoid the short-range repulsion caused by the antiferromagnetic superexchange coupling along the \hat{x} axis⁶⁰⁻⁶³, which can also be seen clearly in Fig. S3 in SI. Therefore, the non-unitary paired ${}^3B_{2u}$ state induced by the FM spin fluctuations results in the formation of Cooper pairing in monolayered CoSb superconductor. The gap zeros of ${}^3B_{2u}$ state ($k_y = 0$ and $k_y = \pi/a_2$) cross the Fermi surface topologies, shown in Fig. 3(a), leading to intriguing nodal behavior. Additionally, it is interesting to point out that the amplitude of Cooper pair spin polarization $\langle \hat{S}_{\vec{k}} \rangle$ on the counters of Fermi surface topologies displays a periodic modulations and vanishes at the nodal points on the Fermi surface topologies, which are the typical characters of non-unitary pairing superconductivity. The DOS of superconducting state with the non-unitary pairing of ${}^3B_{2u}$ symmetry is also calculated and shown in Fig. 3(b). As is expected, the

V-shaped DOS is clearly visible, qualitatively consistent with the experimentally observed STS spectra⁴⁷.

Conclusion. By performing the group theory analysis and the first-principles calculations, we systemically study the electronic and magnetic properties in the monolayered orthorhombic CoSb superconductor, and find the normal state of CoSb to be a half metal with the easy axis of FM magnetization along the \hat{y} axis lying in the basal plane, suggesting the orthorhombic CoSb as a candidate of non-unitary superconductor in which only spin-down electrons are responsible for the Cooper pairing. In the strong-coupling approximation, we suggest the pairing symmetry of CoSb to be a triplet pairing with the irreducible representations of ${}^3B_{2u}$ that displays intriguing nodal points and non-zero periodic modulation of Cooper pair spin polarization on the Fermi surface topologies. While further measurements are also necessary to solidify such symmetry compatible superconducting order parameter and pairing mechanism, these findings imply the novel coexistence of FM and superconducting orders in CoSb and the enhancement of exotic spin polarized Cooper pairing by FM spin fluctuations driving in a triplet superconductor.

Methods

The first-principles calculations

The first-principles calculations are performed using the all-electron full potential linear augmented plane wave method⁶⁴ as implemented in the WIEN2k code⁶⁵. The exchange-correlation potential is calculated using the generalized gradient approximation as proposed by Perdew, Burke, and Ernzerhof⁶⁶. Although the conduction electrons mainly originated from the light atoms of cobalt have a weak spin-orbit coupling, consistent with the group analysis, the heavy mediated anion of antimony has a strong spin-orbit coupling, whose strength is proportional to Z^4 (where Z is the atomic number; $Z = 51$ for Sb)⁶⁷, leading to a significant changes of the overlapped wave functions between the Co $3d$ and Sb $5p$ orbitals⁵⁷. Therefore, the spin-orbit coupling is included with the second variational method throughout the calculations. Furthermore, a 3000 \vec{k} -point is chosen to ensure the calculation with an accuracy of 10^{-5} eV, and all structural parameters (lattice constants, $a_1 = 5.92$ Å and $a_2 = 3.24$ Å, as well as internal coordinates) are performed using the values of experimental crystal structure⁴⁷ shown in Fig. 1(a). To reduce the interaction between

neighboring layers of CoSb, a vacuum slab of 15 Å along the \hat{z} axis is introduced.

Acknowledgements

This work was supported by the National Natural Science Foundation of China (Grant No. 11927807) and the Natural Science Foundation of Shanghai of China (Grant Nos. 19ZR1402600 and 20DZ1100604). W. L. also acknowledges the start-up funding from Fudan University.

Author Contributions

W.L. conceived the project; T.Y., M.Z., and X.W. performed the theoretical calculations; W.L. and X.X. wrote the paper; W.L. and W.J. revised the paper.

Additional Information

Competing financial interests: The authors declare no competing financial interests.

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Figures

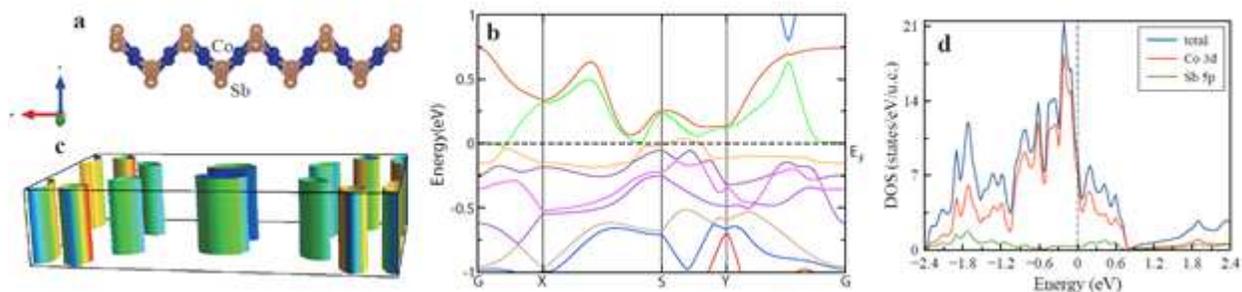


Figure 1

The crystal structure and electronic structure of monolayered CoSb. (a) The schematic illustration of the crystal structure of monolayered orthorhombic CoSb. (b) The electronic band structure and (c) the corresponding Fermi surface topologies for the NM state of monolayered CoSb. (d) The total DOS and PDOS on Co 3d and Sb 5p orbitals for the NM state of monolayered CoSb. The Fermi energies are set to zero.

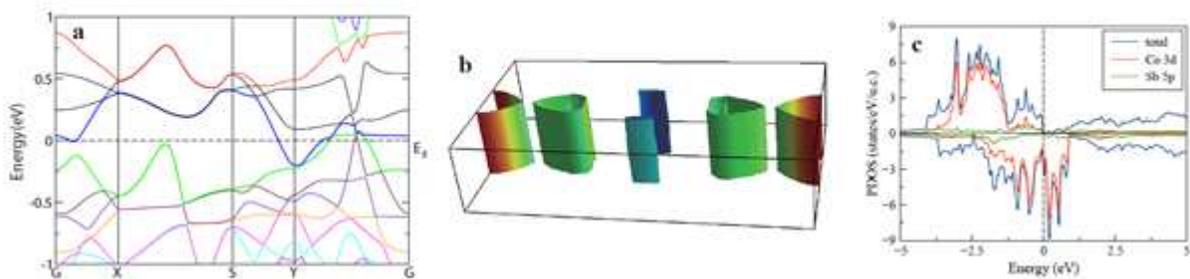


Figure 2

The magnetic structure of monolayered CoSb. (a) The electronic band structure and (b) the corresponding Fermi surface topologies for the FM state of monolayered CoSb. (d) The PDOS on the spin-up and spin-down species of total, Co 3d, and Sb 5p orbitals for the FM state of monolayered CoSb. The Fermi energies are set to zero.

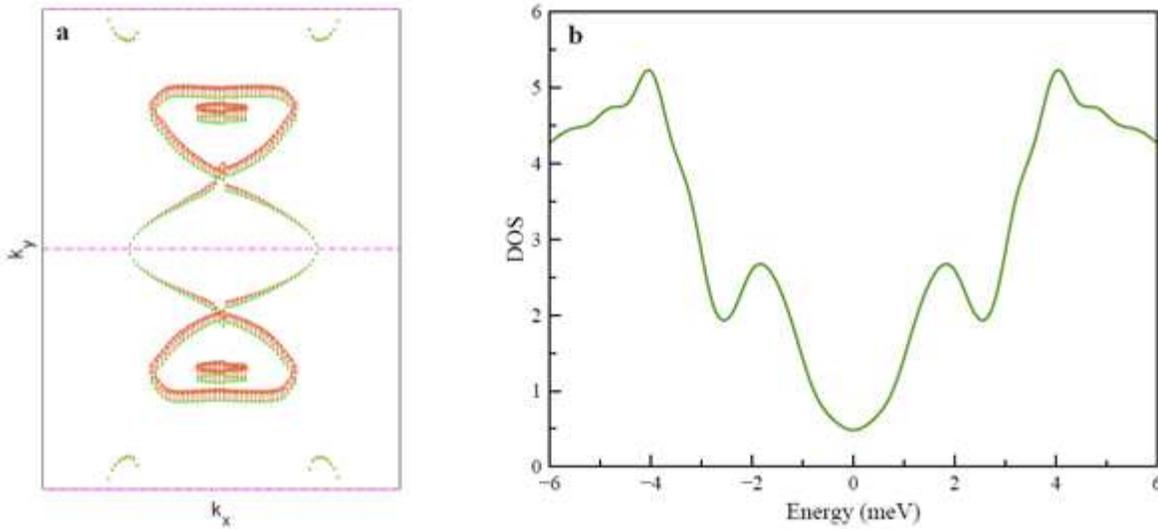


Figure 3

The superconducting properties of monolayered CoSb. (a) A schematic plot for the gap nodal structure of non-unitary pairing on the Fermi surface topologies. The green dotted lines denote the Fermi surface topology of monolayered CoSb, and the magenta dashed lines denote the zero gap value of the order parameter $d(\mathbf{k}) = (1; \pm i; 0) \sin(k_y a^2)$ with the irreducible representation of $3B_2u$. The vector plot of Cooper pair spin polarization $\mathbf{h} \wedge \mathbf{S}_{\mathbf{k}i}$ is also shown on the counters of Fermi surface topologies. (b) The DOS as a function of energy for the non-unitary superconducting state. The parameter of pairing amplitude is set as $\Delta_0 = 5$ meV.

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