

Ni-Intercalation-Induced Topological Nodal Line States and Superconductivity in NiTe

Xin Liang, Ding-Fu Shao,* Run Lv, Rui-Chun Xiao, Hong-Yan Lv, Wen-Jian Lu,* and Yu-Ping Sun



Cite This: *J. Phys. Chem. C* 2023, 127, 4303–4309



Read Online

ACCESS |



Metrics & More

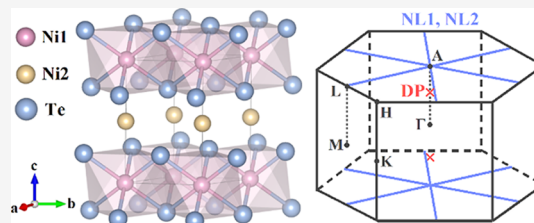


Article Recommendations



Supporting Information

ABSTRACT: Based on symmetry analyses and first-principles calculations, we report the predictions of topological fermions and superconductivity in Ni-intercalated transition metal chalcogenide NiTe. The self-intercalation of Ni introduces nonsymmorphic symmetry operations, protecting a pair of Dirac points and three intersecting Dirac nodal lines near Fermi energy level (E_F), which generate spin-textured surface states across E_F . Moreover, the Ni-intercalation strongly enhances electron–phonon coupling in NiTe and makes it an anisotropic Bardeen–Cooper–Schrieffer superconductor with a full superconducting gap and a critical temperature $T_c \sim 1.5$ K. The coexistence of topological surface states and superconductivity implies that NiTe is a potential material platform for exploring topological superconductivity.



INTRODUCTION

Topological quantum materials have recently become a promising platform for the discovery of novel phenomena with the exotic interplay between the electron, spin, and orbital degrees of freedom.^{1,2} These materials can support nontrivial band crossings at discrete points in the momentum space resembling the Dirac and Weyl fermions known from high-energy physics,^{3–5} or quasiparticles do not have an analogy in high-energy physics,^{6,7} such as the nodal lines^{8–10} and their exotic connections.^{11–15} The topologies of these fermionic excitations result in spin-textured surface/edge states, offering opportunities for exploring solutions to challenging problems in condensed matter physics. One typical example is the topological superconductivity that obeys non-Abelian statistics and is the key to quantum computing.^{16,17} So far, the proof of the existence of topological superconductivity is still inclusive. Among the proposals to solve this problem,^{18–22} one promising direction is to utilize the superconducting topological semimetals, where the interaction of helical surface states and superconducting Cooper pairs in the same material results in the Majorana fermions on the surfaces.^{21,22} This requires the exploration of realistic material platforms hosting both nontrivial topology and superconductivity at a finite temperature.

Recently, transition metal dichalcogenides (TMDs) family has attracted increasing interest due to the advantages of designing functionalities. Although the Dirac and Weyl fermions have been observed in TMDs,^{23–26} the topological surface states associated with these fermions are restricted to a narrow energy window near the Dirac or Weyl points, where the low density of states is difficult to support a strong electron–phonon coupling (EPC) and hence the superconductivity. On the other hand, the topological Dirac nodal lines are usually dispersive and accompanied by the metallic phases within a wide energy

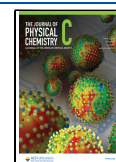
window, supporting exotic surface states and a sizable density of states promising for topological superconductivity. However, the relativistic Dirac nodal lines are rarely found in TMDs, since most metallic TMDs usually have the 1T-phase, which hosts the symmorphic space groups and hence cannot protect the fourfold degeneracy along lines in the momentum space.^{27,28} It is interesting if one can find a way to introduce nonsymmorphic symmetry into TMDs to protect both Dirac points and Dirac nodal lines, and modulate the electronic structure for a strong EPC to support superconductivity at a finite temperature.

In this work, we demonstrate based on symmetry analyses and first-principles density functional theory calculations, the Dirac points, Dirac nodal lines, and superconductivity simultaneously introduced in Ni-intercalated Ni_2Te_2 (i.e., NiTe). For NiTe, Ni-intercalation yields a nonsymmorphic space group $P6_3/mmc$ hosting a glide symmetry and a screw symmetry, which protect three straight Dirac nodal lines across the Fermi energy level (E_F) and a pair of Dirac nodal points near E_F , respectively. Moreover, the remodulation of the electronic structure by Ni-intercalation results in a strong EPC. With the spin-textured surface states induced by the topological fermions and the predicted superconducting critical temperature (T_c) of ~ 1.5 K, the self-intercalated NiTe is a potential candidate for realizing topological superconductivity.

Received: November 21, 2022

Revised: January 26, 2023

Published: February 20, 2023



METHODS

The first-principles calculations were performed based on density functional theory (DFT)²⁹ as implemented in the Vienna ab initio simulation package (VASP).^{30,31} The generalized gradient approximation (GGA) according to the Perdew–Burke–Ernzerhof (PBE)³² type was used to describe the exchange–correlation function. The plane-wave kinetic cutoff energy was set as 500 eV in all first-principles calculations. Both the lattice parameters and atomic positions were fully optimized until the total energy and force convergence criteria were set to be 10^{-8} eV and 0.001 eV/Å, respectively. The Brillouin zone (BZ) was sampled with $12 \times 12 \times 8$ Γ -centered k mesh. Van der Waals (vdW) interactions were treated by using Grimme's DFT-D2 of the semiempirical method.³³ Since these materials contain transition metal elements (Ni), the possible correlation effect of the d orbitals was tested using the GGA+ U method,^{34,35} which yielded almost the same results at E_F as that from the GGA calculations (Figure S1). Spin-orbit coupling (SOC) was included in all the electronic calculations. The irreducible representations of electronic eigenstates were obtained via an in-house code and the software package irvsp.³⁶ The Fermi surfaces were calculated by Wannier90 code³⁷ utilizing the maximally localized Wannier functions^{38,39} and visualized by the program XCrySDen.⁴⁰ The topological surface states and associated spin textures were calculated by using the Wannier Tools package.⁴¹

Calculations of EPC were performed based on DFT and density functional perturbation theory (DFPT) as implemented in the QUANTUM ESPRESSO package.⁴² The cutoff energies of the charge density and wave functions were set as 500 and 50 Ry, respectively. The BZ was sampled on a $12 \times 12 \times 8$ mesh of k -points, ensuring that the convergence criterion for energy (force) is less than 10^{-6} Ry (10^{-5} Ry/Å). The Gaussian smearing method was used to calculate the charge density with a smearing parameter of $\sigma = 0.005$ Ry. For EPC calculations, where a denser $24 \times 24 \times 16$ k -points grid and a $6 \times 6 \times 4$ q -points grid were employed. We employ the Superconducting-Toolkit package^{43,44} based on the DFT for superconductors (SCDFT)^{45,46} to calculate the momentum-resolved superconducting gap and EPC strength.

RESULTS AND DISCUSSION

1T-NiTe₂ is a layered vdW compound hosting a CdI₂-type hexagonal structure. A pair of type-II Dirac points was found in this material protected by the symmorphic space group of $P\bar{3}m1$.^{28,47} The superconductivity is absent in NiTe₂ due to the weak EPC.^{48,49} It was found that the isolated Ni atoms can be intercalated into the vdW gap of NiTe₂, forming a centrosymmetric and nonmagnetic NiTe. As shown in Figure 1, the intercalated Ni atom (denoted as Ni2) locates at the center of the two nearest original Ni atoms (denoted as Ni1) in the vertical direction. The nonsymmorphic space group $P6_3/mmc$ of NiTe contains a twofold screw axis $S_{2z} = \{C_{2z} | t_z\}$ and a glide mirror $G_z = \{M_z | t_z\}$ which connect Ni1 and Ni2 atoms, where C_{2z} is a twofold rotation around the z -axis, M_z is a mirror perpendicular to the z -axis, and t_z is a half-unit-cell translation along the z -direction. Moreover, it has a threefold rotation C_{3z} and three mirrors $M_{||}$ parallel to the z -axis, as depicted in Figure 1.

Figure 2a shows the band structure of NiTe. Four bands are crossing E_F , leading to a complex Fermi surface that consists of two-hole pockets around the A point, a lantern-shaped hexagonal hole pocket in the center of BZ, a gear-shaped

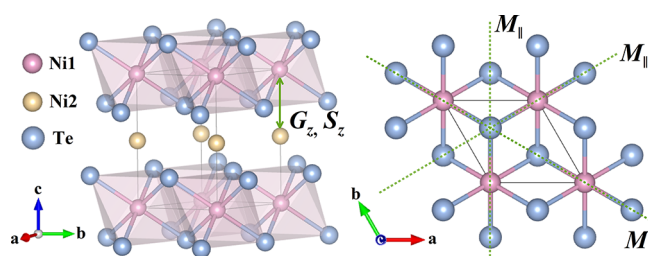


Figure 1. Side view and top view of the crystal structure of NiTe. Ni1 represents the Ni atoms of the original NiTe₂ sandwich layer, and Ni2 represents the intercalated Ni atoms. The symmetric operations such as the glide mirror G_z and screw axis S_z , as well as the mirror $M_{||}$ parallel to the z -axis are marked.

electron pocket at the boundary of the $k_z = 0$ plane, and six small electron pockets around the K point (Figures 2d and S2). Projected density of states (PDOS) suggests that the bands close to E_F are mainly contributed by Ni-3d orbitals and Te-5p orbitals, and the contribution of Ni-3d orbital at E_F is significantly larger than that of Te-5p orbitals, as shown in Figure 2c. Comparing the electronic structure of NiTe with that of NiTe₂ (Figure S3), we find that the intercalation of Ni significantly enhances the Ni-3d electronic state and the p - d orbital hybridization at E_F in NiTe.

The nonsymmorphic symmetry induced by Ni-intercalation brings in nontrivial band crossings in NiTe. Each band is doubly degenerate in BZ, which is enforced by the inversion and time reversal symmetry. There is a band crossing located slightly above E_F in the Γ –A direction ($k_z > 0$), forming a fourfold degenerate Dirac point (denoted as DP in Figure 2b,e). And there is another Dirac point located at the same energy in the Γ –A direction for $k_z < 0$ by symmetry. This is due to the line of $k_x = k_y = 0$ is invariant to the S_{2z} symmetry, which can protect the fourfold degeneracy of the bands.^{5,15} We denote the two bands forming the Dirac point in the Γ –A direction by different colors and their irreducible representations in Figure 2b. The band crossing near E_F is inevitable, since the Δ_7 (yellow) and Δ_8 (green) bands belong to different irreducible representations. We also find that the band crossing leading to this Dirac point is dominated by Te-5p orbitals (Figure S4), consistent with the case in other TMDs where the band inversions are usually from the chalcogen p orbitals.^{28,50}

There are four isolated doubly degenerate bands in the Γ –A direction that merge into 2 fourfold degenerate bands along the A–L direction in $k_z = 0.5$ plane near E_F , forming the Dirac nodal lines (denoted as NL1 and NL2 in Figure 2b,e). This is also reflected by the difference in eigenvalues between the doubly degenerate bands near E_F in $k_z = 0.5$ plane, where the eigenvalue difference is absent along three A–L directions (Figure S5). These three intersecting Dirac nodal lines are enforced by G_z , $M_{||}$, and C_{3z} , as the anticommutation relation $\{M_{||}, G_z\} = 0$ for $k_x = 0$ and $k_z = 0.5$ results in a Dirac nodal line in this direction, and the application of C_{3z} operation to this Dirac nodal line generates additional two Dirac nodal lines for $k_x = \pm\sqrt{3}k_y$ and $k_z = 0.5$, as shown in Figure 2e.

A typical property of the topological fermions is the exotic surface states and Fermi arcs. Here, we show the surface states for the (010) surface of NiTe in Figure 3a,b. For both Ni- and Te-terminated surfaces, we find that there are surface states connecting a pair of Dirac points close to E_F , and surface states crossing E_F appear between Dirac nodal lines in the $\bar{A}$ – $\bar{L}$ – $\bar{A}$ direction. These surface states carry exotic spin textures as

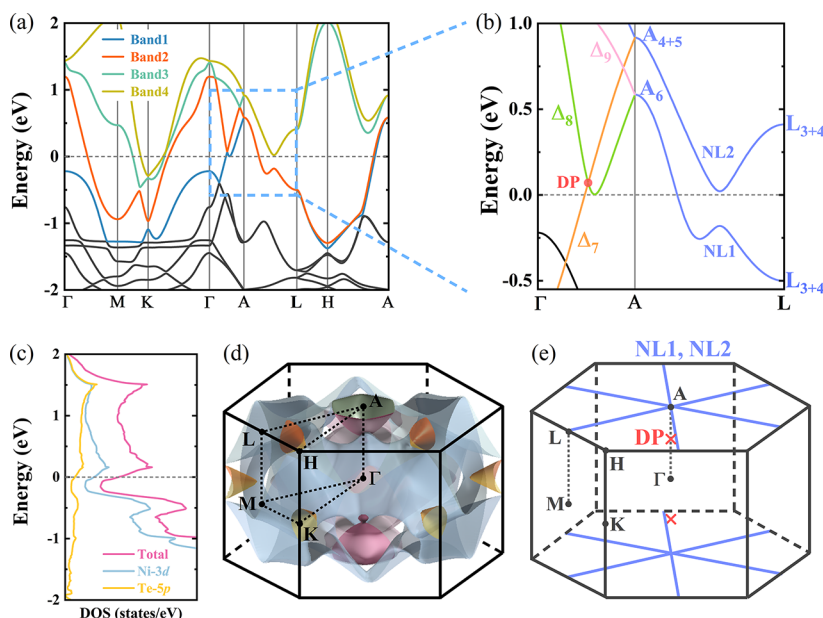


Figure 2. Electronic structure of NiTe. (a) Band structure for NiTe. The four energy bands crossing E_F are marked with different colors. (b) Zoom-in band structure near E_F along the Γ –A–L direction. The Dirac point, Dirac nodal lines, and irreducible representations of bands are indicated. (c) Projected density of states for NiTe. (d) Fermi surfaces of four bands crossing E_F . The high-symmetry points are marked. (e) Schematic figure describing the distribution of Dirac points and nodal lines in momentum space. High-symmetry points are marked.

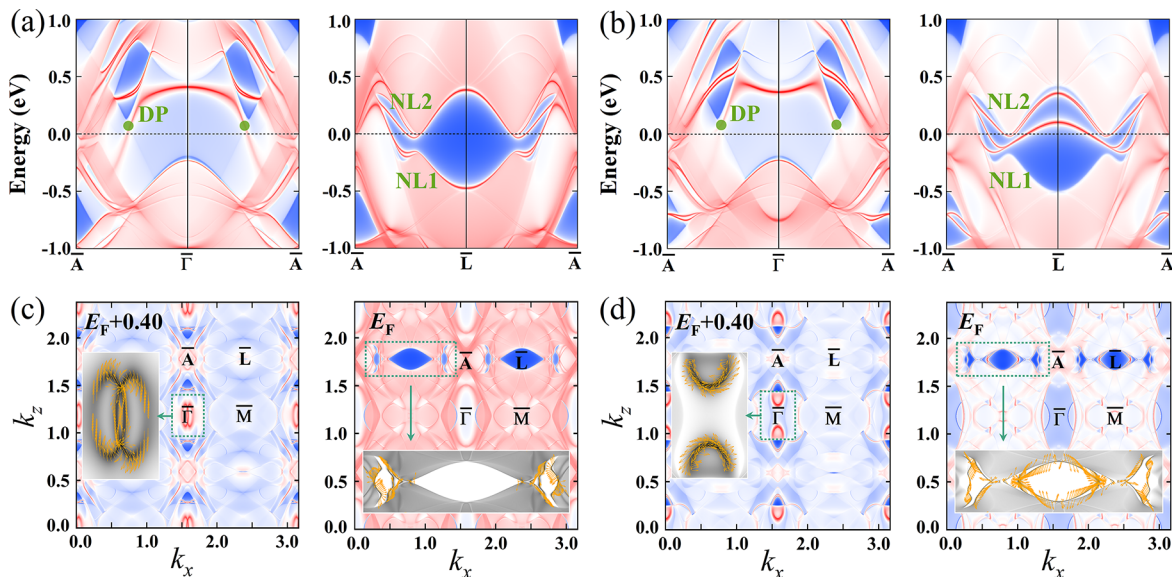


Figure 3. Calculated the Ni-terminated (a) and Te-terminated (b) (010)-projected surface state spectra of NiTe with SOC along the different directions. Bright-colored red lines mean the topological surface states. Constant energy slices on Ni-terminated (c) and Te-terminated (d) surfaces of the (010) slab. Here, we include the constant energy slices for the chemical potential μ of 0 and 0.4 eV, since the surface states generated by the Dirac points are concealed by the bulk state for $\mu = 0$ eV but can be clearly seen for $\mu = 0.4$ eV. The yellow arrows in the insets denote the corresponding spin textures of topological surface states. The k -space range is defined by the green dotted box.

evidenced by the surface Fermi arc calculation in Figure 3c,d. Spin-helical topological surface states propagating along opposite directions are with opposite spin polarizations. We also find that the spin textures of surface states crossing E_F generated between Dirac nodal lines exhibit chirality, which can be seen in Figure S6 of the zoomed-in spin textures. The chiral spin textures, together with conventional s -wave interactions, lead to topological superconductivity and non-Abelian Majorana fermions.⁵¹ The surface states of NiTe prove the nontrivial topologies of the Dirac points and the Dirac nodal lines, which

can be observed easily in angle-resolved photoemission spectroscopy (ARPES) experiments and may be reflected in the transport properties.

Next, we investigate the potential superconductivity of NiTe. Figure 4a shows the phonon dispersion of NiTe, where the absence of imaginary frequencies in the whole BZ indicates the dynamical stability of NiTe. The strength of EPC can be estimated by calculating the EPC constant $\lambda(\omega)$ as

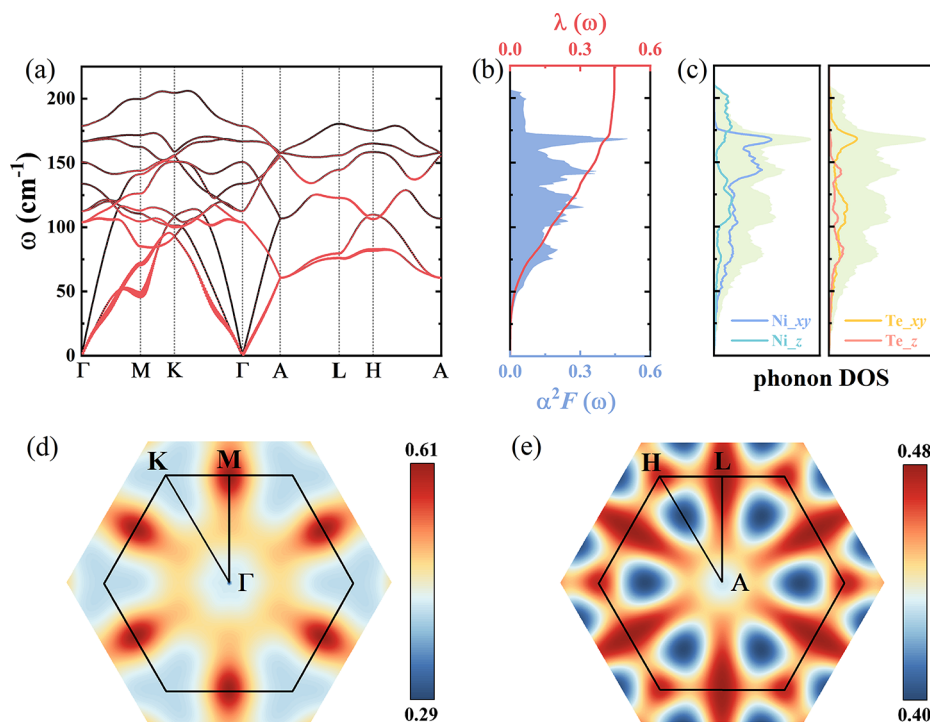


Figure 4. EPC properties of NiTe with SOC. (a) Phonon dispersions weighted by the magnitude of the EPC strength. (b) Eliashberg spectral function $\alpha^2F(\omega)$ and the integrated strength of EPC $\lambda(\omega)$. (c) Phonon density of states (PhDOS) in NiTe. The green-shaded zone indicates the total PhDOS. (d,e) Integrated EPC distributions for the plane of $q_z = 0$ (d) and the plane of $q_z = 0.5$ (e).

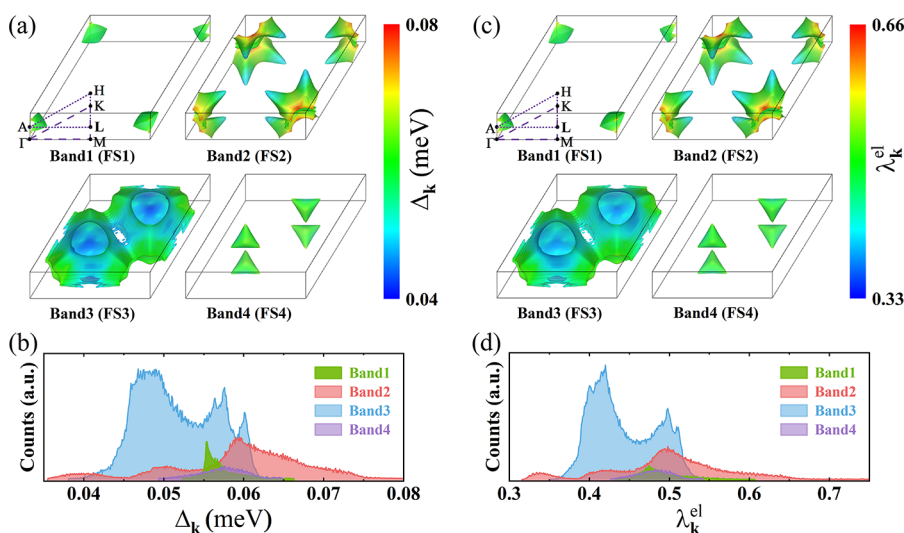


Figure 5. (a) Momentum-resolved superconducting gap Δ_k on different sheets of the Fermi surface for NiTe with SOC. (b) Energy distribution of the superconducting gap Δ_k . (c) Momentum-resolved EPC strength λ_k^{el} on different sheets of the Fermi surface for NiTe with SOC. (d) Distribution of the EPC strength λ_k^{el} by magnitude.

$$\lambda(\omega) = \sum_{\mathbf{q}\nu} \lambda_{\mathbf{q}\nu} = 2 \int_0^\omega \frac{\alpha^2F(\omega)}{\omega} d\omega \quad (1)$$

where ω is the phonon frequency, $\lambda_{\mathbf{q}\nu}$ is the EPC constant contributed by the ν th mode at the wave vector $\mathbf{q}$, and $\alpha^2F(\omega)$ is the Eliashberg spectral function

$$\alpha^2F(\omega) = \frac{1}{2\pi N(E_F)} \sum_{\mathbf{q}\nu} \delta(\omega - \omega_{\mathbf{q}\nu}) \frac{\gamma_{\mathbf{q}\nu}}{\hbar\omega_{\mathbf{q}\nu}} \quad (2)$$

where $N(E_F)$ is the electronic DOS at E_F , $\gamma_{\mathbf{q}\nu}$ is the phonon linewidth defined by

$$\gamma_{\mathbf{q}\nu} = 2\pi\omega_{\mathbf{q}\nu} \sum_{ij} \int \frac{d\mathbf{k}}{\Omega_{\text{BZ}}} |g_{\mathbf{q}\nu}(\mathbf{k}, i, j)|^2 \times \delta(\epsilon_{\mathbf{k},i} - E_F) \delta(\epsilon_{\mathbf{k}+\mathbf{q},j} - E_F) \quad (3)$$

where $g_{\mathbf{q}\nu}$ is the EPC matrix element. We decorate the magnitude of $\lambda_{\mathbf{q}\nu}$ in the phonon dispersion (Figure 4a), which is estimated by

$$\lambda_{qv} = \frac{\gamma_{qv}}{\pi \hbar N(E_F) \omega_{qv}^2} \quad (4)$$

Obviously, a low ω_{qv} can result in a strong EPC. Therefore, several soft acoustic modes around the M, L, and H points significantly contribute to the total EPC (Figure 4a). This can be also seen in the distributions of total λ in the $q_z = 0$ and 0.5 planes of the BZ (Figure 4d,e).

We predict the superconducting transition temperature T_c of NiTe based on the Allen–Dynes–modified McMillan formula:⁵²

$$T_c = \frac{\omega_{\log}}{1.2} \exp\left(-\frac{1.04(1 + \lambda)}{\lambda - \mu^* - 0.62\lambda\mu^*}\right) \quad (5)$$

the logarithmically averaged characteristic phonon frequency $\omega_{\log}$ is defined as

$$\omega_{\log} = \exp\left(\frac{2}{\lambda} \int \frac{d\omega}{\omega} \alpha^2 F(\omega) \log \omega\right) \quad (6)$$

We calculate T_c by using different Coulomb pseudopotential μ^* values to evaluate the superconductivity (Figure S7) and find that T_c decreased gradually with increasing μ^* . Here, we adopt a typical μ^* value of 0.1.^{53,54} The calculated $\lambda = 0.48$ and $\omega_{\log} = 149.3$ K resulting in T_c of 1.5 K for NiTe. We note the vibration of Ni atoms contributed mostly to the phonon density of states (PhDOS) of NiTe (Figure 4c). Since PhDOS and $\alpha^2 F(\omega)$ (Figure 4b) have similar shapes, we conclude that a larger Ni concentration of NiTe compared to that of nonsuperconducting NiTe₂ directly results in stronger EPC for observable superconductivity in the self-intercalated NiTe.

Figure 5a plots the momentum-resolved superconducting gap Δ_k on four sheets of the Fermi surface (denoted as FS_{*i*} where *i* = 1, 2, 3, 4) for NiTe. We find Δ_k is finite over all Fermi sheets, indicating that the Fermi surface is fully gapped below the critical temperature. The distributions of Δ_k on FS1 and FS4 are nearly isotropic. On the other hand, Δ_k on FS2 and FS3 are highly anisotropic and vary over the wide range of 0.035–0.080 and 0.038–0.063 meV, respectively (Figure 5b). We find Δ_k on FS2 is significantly larger than that on other sheets. The largest Δ_k occurs at the parts of FS2 with the smallest radius $\eta_{\parallel} = \sqrt{k_x^2 + k_y^2}$ (Figure 5a). Figure 5c,d shows the distribution of electronic strength λ_k^{el} on the Fermi surface, which is consistent with that for Δ_k shown in Figure 5a. Therefore, NiTe is an anisotropic Bardeen–Cooper–Schrieffer (BCS) superconductor with a full superconducting gap.

The coexistence of the topological surface states and superconductivity in NiTe implies the possibility of topological superconductivity. Below superconducting T_c , the superconducting gap is opened on all the Fermi surfaces, and thus, topological superconductivity may be induced in the topological surface states by the proximity effect. In this situation, helically spin-polarized electrons on the topological surface states can form superconducting pairs and bound Majorana fermions in the vortices.^{21,22} The convenient sample preparation and the finite superconducting T_c of NiTe imply the possible experimental verification of the topological superconductivity under a normal experimental condition.

CONCLUSIONS

In summary, based on the symmetry analyses and first-principles calculations, we predict that the self-intercalated NiTe hosts simultaneously topological fermions and superconductivity.

NiTe is prepared by inserting a Ni atom into the vdW gap of NiTe₂, where the self-intercalation of Ni introduces non-symorphic symmetry operations, protecting topological Dirac points and Dirac nodal lines near E_F which generate spin-textured surface states. Moreover, Ni-intercalation strongly enhances EPC, making NiTe an anisotropic BCS superconductor with a full superconducting gap and a finite T_c of ~ 1.5 K. The coexistence of the topological surface states and superconductivity implies that NiTe is a potential material candidate to explore the topological superconductivity. We hope that our predictions will stimulate experimental investigations of self-intercalated TMDs and the associated phenomena.

ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available free of charge at <https://pubs.acs.org/doi/10.1021/acs.jpcc.2c08143>.

More details on the Fermi surfaces, electronic structure, nodal lines, surface states, and superconductivity (PDF)

AUTHOR INFORMATION

Corresponding Authors

Ding-Fu Shao – Key Laboratory of Materials Physics, Institute of Solid State Physics, HFIPS, Chinese Academy of Sciences, Hefei 230031, China; orcid.org/0000-0002-2732-4131; Email: dfshao@issp.ac.cn

Wen-Jian Lu – Key Laboratory of Materials Physics, Institute of Solid State Physics, HFIPS, Chinese Academy of Sciences, Hefei 230031, China; Email: wjlu@issp.ac.cn

Authors

Xin Liang – Key Laboratory of Materials Physics, Institute of Solid State Physics, HFIPS, Chinese Academy of Sciences, Hefei 230031, China; University of Science and Technology of China, Hefei 230026, China; orcid.org/0000-0002-5657-8704

Run Lv – Key Laboratory of Materials Physics, Institute of Solid State Physics, HFIPS, Chinese Academy of Sciences, Hefei 230031, China; University of Science and Technology of China, Hefei 230026, China

Rui-Chun Xiao – Institute of Physical Science and Information Technology, Anhui University, Hefei 230601, China

Hong-Yan Lv – School of Physics, Hefei University of Technology, Hefei 230009, China

Yu-Ping Sun – Key Laboratory of Materials Physics, Institute of Solid State Physics, HFIPS, Chinese Academy of Sciences, Hefei 230031, China; High Magnetic Field Laboratory, HFIPS, Chinese Academy of Sciences, Hefei 230031, China; Collaborative Innovation Center of Microstructures, Nanjing University, Nanjing 210093, China

Complete contact information is available at:

<https://pubs.acs.org/doi/10.1021/acs.jpcc.2c08143>

Notes

The authors declare no competing financial interest.

ACKNOWLEDGMENTS

This work was supported by the National Key R&D Program of China under Contract No. 2022YFA1403203, the National Nature Science Foundation of China under Contract No. U2032215, No. 12274411, and No. 12274412. The calculations were performed at Hefei Advanced Computing Center.

REFERENCES

- (1) Chen, Y. L.; Analytis, J. G.; Chu, J.-H.; Liu, Z. K.; Mo, S.-K.; Qi, X. L.; Zhang, H. J.; Lu, D. H.; Dai, X.; Fang, Z.; et al. Experimental realization of a three-dimensional topological insulator; Bi_2Te_3 . *Science* **2009**, *325*, 178–181.
- (2) Keimer, B.; Moore, J. E. The physics of quantum materials. *Nat. Phys.* **2017**, *13*, 1045–1055.
- (3) Wan, X.; Turner, A. M.; Vishwanath, A.; Savrasov, S. Y. Topological semimetal and Fermi-arc surface states in the electronic structure of pyrochlore iridates. *Phys. Rev. B* **2011**, *83*, No. 205101.
- (4) Liu, Z. K.; Zhou, B.; Zhang, Y.; Wang, Z. J.; Weng, H. M.; Prabhakaran, D.; Mo, S.-K.; Shen, Z. X.; Fang, Z.; Dai, X.; et al. Discovery of a three-dimensional topological Dirac semimetal; Na_3Bi . *Science* **2014**, *343*, 864–867.
- (5) Armitage, N. P.; Mele, E. J.; Vishwanath, A. Weyl and Dirac semimetals in three-dimensional solids. *Rev. Mod. Phys.* **2018**, *90*, No. 015001.
- (6) Yang, B.-J.; Nagaosa, N. Classification of stable three-dimensional Dirac semimetals with nontrivial topology. *Nat. Commun.* **2014**, *5*, 4898.
- (7) Weng, H.; Fang, C.; Fang, Z.; Dai, X. Topological semimetals with triply degenerate nodal points in θ -phase tantalum nitride. *Phys. Rev. B* **2016**, *93*, No. 241202(R).
- (8) Fang, C.; Chen, Y.; Kee, H.-Y.; Fu, L. Topological nodal line semimetals with and without spin-orbital coupling. *Phys. Rev. B* **2015**, *92*, No. 081201(R).
- (9) Weng, H.; Liang, Y.; Xu, Q.; Yu, R.; Fang, Z.; Dai, X.; Kawazoe, Y. Topological node-line semimetal in three-dimensional graphene networks. *Phys. Rev. B* **2015**, *92*, No. 045108.
- (10) Yu, R.; Weng, H.; Fang, Z.; Dai, X.; Hu, X. Topological node-line semimetal and Dirac semimetal state in antiperovskite Cu_3PdN . *Phys. Rev. Lett.* **2015**, *115*, No. 036807.
- (11) Wang, S.-S.; Liu, Y.; Yu, Z.-M.; Sheng, X.-L.; Yang, S. A. Hourglass Dirac chain metal in rhenium dioxide. *Nat. Commun.* **2017**, *8*, 1844.
- (12) Chen, W.; Lu, H.-Z.; Hou, J.-M. Topological semimetals with a double-helix nodal link. *Phys. Rev. B* **2017**, *96*, No. 041102(R).
- (13) Feng, X.; Yue, C.; Song, Z.; Wu, Q.; Wen, B. Topological Dirac nodal-net fermions in AlB_2 -type TiB_2 and ZrB_2 . *Phys. Rev. Mater.* **2018**, *2*, No. 014202.
- (14) Bzduszek, T.; Wu, Q.; Rüegg, A.; Sigrist, M.; Soluyanov, A. A. Nodal-chain metals. *Nature* **2016**, *538*, 75–78.
- (15) Shao, D.-F.; Zhang, S.-H.; Dang, X.; Tsymbal, E. Y. Tunable two-dimensional Dirac nodal nets. *Phys. Rev. B* **2018**, *98*, No. 161104(R).
- (16) Kitaev, A. Y. Fault-tolerant quantum computation by anyons. *Ann. Phys.* **2003**, *303*, 2–30.
- (17) Nayak, C.; Simon, S. H.; Stern, A.; Freedman, M.; Sarma, S. D. Non-Abelian anyons and topological quantum computation. *Rev. Mod. Phys.* **2008**, *80*, 1083.
- (18) Fu, L.; Berg, E. Odd-parity topological superconductors: theory and application to $\text{Cu}_x\text{Bi}_2\text{Se}_3$. *Phys. Rev. Lett.* **2010**, *105*, No. 097001.
- (19) Nadj-Perge, S.; Drozdov, I. K.; Li, J.; Chen, H.; Jeon, S.; Seo, J.; MacDonald, A. H.; Bernevig, B. A.; Yazdani, A. Observation of Majorana fermions in ferromagnetic atomic chains on a superconductor. *Science* **2014**, *346*, 602–607.
- (20) Sun, H.-H.; Zhang, K.-W.; Hu, L.-H.; Li, C.; Wang, G.-Y.; Ma, H.-Y.; Xu, Z.-A.; Gao, C.-L.; Guan, D.-D.; Li, Y.-Y.; et al. Majorana zero mode detected with spin selective Andreev reflection in the vortex of a topological superconductor. *Phys. Rev. Lett.* **2016**, *116*, No. 257003.
- (21) Guan, S.-Y.; Chen, P.-J.; Chu, M.-W.; Sankar, R.; Chou, F.; Jeng, H.-T.; Chang, C.-S.; Chuang, T.-M. Superconducting topological surface states in the noncentrosymmetric bulk superconductor PbTaSe_2 . *Sci. Adv.* **2016**, *2*, No. e1600894.
- (22) Zhang, P.; Yaji, K.; Hashimoto, T.; Ota, Y.; Kondo, T.; Okazaki, K.; Wang, Z.; Wen, J.; Gu, G. D.; Ding, H.; et al. Observation of topological superconductivity on the surface of an iron-based superconductor. *Science* **2018**, *360*, 182–186.
- (23) Deng, K.; Wan, G.; Deng, P.; Zhang, K.; Ding, S.; Wang, E.; Yan, M.; Huang, H.; Zhang, H.; Xu, Z.; et al. Experimental observation of topological Fermi arcs in type-II Weyl semimetal MoTe_2 . *Nat. Phys.* **2016**, *12*, 1105–1110.
- (24) Li, P.; Wen, Y.; He, X.; Zhang, Q.; Xia, C.; Yu, Z.-M.; Yang, S. A.; Zhu, Z.; Alshareef, H. N.; Zhang, X.-X. Evidence for topological type-II Weyl semimetal WTe_2 . *Nat. Commun.* **2017**, *8*, 2150.
- (25) Yan, M.; Huang, H.; Zhang, K.; Wang, E.; Yao, W.; Deng, K.; Wan, G.; Zhang, H.; Arita, M.; Yang, H.; et al. Lorentz-violating type-II Dirac fermions in transition metal dichalcogenide PtTe_2 . *Nat. Commun.* **2017**, *8*, 257.
- (26) Xiao, R. C.; Gong, P. L.; Wu, Q. S.; Lu, W. J.; Wei, M. J.; Li, J. Y.; Lv, H. Y.; Luo, X.; Tong, P.; Zhu, X. B.; et al. Manipulation of type-I and type-II Dirac points in PdTe_2 superconductor by external pressure. *Phys. Rev. B* **2017**, *96*, No. 075101.
- (27) Zhang, K.; Yan, M.; Zhang, H.; Huang, H.; Arita, M.; Sun, Z.; Duan, W.; Wu, Y.; Zhou, S. Experimental evidence for type-II Dirac semimetal in PtSe_2 . *Phys. Rev. B* **2017**, *96*, No. 125102.
- (28) Mukherjee, S.; Jung, S. W.; Weber, S. F.; Xu, C.; Qian, D.; Xu, X.; Biswas, P. K.; Kim, T. K.; Chapon, L. C.; Watson, M. D.; et al. Fermi-crossing Type-II Dirac fermions and topological surface states in NiTe_2 . *Sci. Rep.* **2020**, *10*, 12957.
- (29) Hohenberg, P.; Kohn, W. Inhomogeneous electron gas. *Phys. Rev.* **1964**, *136*, B864.
- (30) Kresse, G.; Hafner, J. *Ab initio* molecular dynamics for liquid metals. *Phys. Rev. B* **1993**, *47*, 558.
- (31) Kresse, G.; Furthmüller, J. Efficient iterative schemes for *ab initio* total-energy calculations using a plane-wave basis set. *Phys. Rev. B* **1996**, *54*, 11169.
- (32) Perdew, J. P.; Burke, K.; Ernzerhof, M. Generalized gradient approximation made simple. *Phys. Rev. Lett.* **1996**, *77*, 3865.
- (33) Grimme, S. Semiempirical GGA-type density functional constructed with a long-range dispersion correction. *J. Comput. Chem.* **2006**, *27*, 1787–1799.
- (34) Anisimov, V. I.; Zaanen, J.; Andersen, O. K. Band theory and Mott insulators: Hubbard U instead of Stoner I . *Phys. Rev. B* **1991**, *44*, 943.
- (35) Dudarev, S. L.; Botton, G. A.; Savrasov, S. Y.; Humphreys, C. J.; Sutton, A. P. Electron-energy-loss spectra and the structural stability of nickel oxide: An LSDA+ U study. *Phys. Rev. B* **1998**, *57*, 1505.
- (36) Gao, J.; Wu, Q.; Persson, C.; Wang, Z. Irvsp: To obtain irreducible representations of electronic states in the VASP. *Comput. Phys. Commun.* **2021**, *261*, No. 107760.
- (37) Mostofi, A. A.; Yates, J. R.; Pizzi, G.; Lee, Y.-S.; Souza, I.; Vanderbilt, D.; Marzari, N. An updated version of wannier90: A tool for obtaining maximally-localised Wannier functions. *Comput. Phys. Commun.* **2014**, *185*, 2309–2310.
- (38) Marzari, N.; Vanderbilt, D. Maximally localized generalized Wannier functions for composite energy bands. *Phys. Rev. B* **1997**, *56*, 12847.
- (39) Souza, I.; Marzari, N.; Vanderbilt, D. Maximally localized Wannier functions for entangled energy bands. *Phys. Rev. B* **2001**, *65*, No. 035109.
- (40) Kokalj, A. Computer graphics and graphical user interfaces as tools in simulations of matter at the atomic scale. *Comput. Mater. Sci.* **2003**, *28*, 155–168.
- (41) Wu, Q.; Zhang, S.; Song, H.-F.; Troyer, M.; Soluyanov, A. A. WannierTools: An open-source software package for novel topological materials. *Comput. Phys. Commun.* **2018**, *224*, 405–416.
- (42) Giannozzi, P.; Baroni, S.; Bonini, N.; Calandra, M.; Car, R.; Cavazzoni, C.; Ceresoli, D.; Chiarotti, G. L.; Cococcioni, M.; Dabo, I.; et al. QUANTUM ESPRESSO: a modular and open-source software project for quantum simulations of materials. *J. Phys.: Condens. Matter* **2009**, *21*, No. 395502.
- (43) Kawamura, M.; Akashi, R.; Tsuneyuki, S. Anisotropic superconducting gaps in $\text{YNi}_2\text{B}_2\text{C}$: A first-principles investigation. *Phys. Rev. B* **2017**, *95*, No. 054506.
- (44) Kawamura, M.; Hizume, Y.; Ozaki, T. Benchmark of density functional theory for superconductors in elemental materials. *Phys. Rev. B* **2020**, *101*, No. 134511.

- (45) Oliveira, L. N.; Gross, E. K. U.; Kohn, W. Density-Functional Theory for Superconductors. *Phys. Rev. Lett.* **1988**, *60*, 2430.
- (46) Lüders, M.; Marques, M. A. L.; Lathiotakis, N. N.; Floris, A.; Profeta, G.; Fast, L.; Continenza, A.; Massidda, S.; Gross, E. K. U. *Ab initio* theory of superconductivity. I. Density functional formalism and approximate functionals. *Phys. Rev. B* **2005**, *72*, No. 024545.
- (47) Xu, C.; Li, B.; Jiao, W.; Zhou, W.; Qian, B.; Sankar, R.; Zhigadlo, N. D.; Qi, Y.; Qian, D.; Chou, F.-C.; et al. Topological type-II Dirac fermions approaching the Fermi level in a transition metal dichalcogenide NiTe_2 . *Chem. Mater.* **2018**, *30*, 4823–4830.
- (48) Zheng, F.; Li, X.-B.; Tan, P.; Lin, Y.; Xiong, L.; Chen, X.; Feng, J. Emergent superconductivity in two-dimensional NiTe_2 crystals. *Phys. Rev. B* **2020**, *101*, No. 100505(R).
- (49) Zhang, J.-F.; Zhao, Y.; Liu, K.; Liu, Y.; Lu, Z.-Y. First-principles study of the crystal structure; electronic structure; and transport properties of NiTe_2 under pressure. *Phys. Rev. B* **2021**, *104*, No. 035111.
- (50) Clark, O. J.; Neat, M. J.; Okawa, K.; Bawden, L.; Marković, I.; Mazzola, F.; Feng, J.; Sunko, V.; Riley, J. M.; Meevasana, W.; et al. Fermiology and superconductivity of topological surface states in PdTe_2 . *Phys. Rev. Lett.* **2018**, *120*, No. 156401.
- (51) Sau, J. D.; Sensarma, R.; Powell, S.; Spielman, I. B.; Sarma, S. D. Chiral Rashba spin textures in ultracold Fermi gases. *Phys. Rev. B* **2011**, *83*, No. 140510(R).
- (52) Allen, P. B.; Dynes, R. C. Transition temperature of strong-coupled superconductors reanalyzed. *Phys. Rev. B* **1975**, *12*, 905.
- (53) Kortus, J.; Mazin, I. I.; Belashchenko, K. D.; Antropov, V. P.; Boyer, L. L. Superconductivity of metallic boron in MgB_2 . *Phys. Rev. Lett.* **2001**, *86*, 4656.
- (54) Calandra, M.; Mauri, F. Charge-density wave and superconducting dome in TiSe_2 from electron-phonon interaction. *Phys. Rev. Lett.* **2011**, *106*, No. 196406.