

Van Hove Singularities, Superconductivity, and the Josephson Diode Effect in NiTe₂ and PdTe₂

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Superconductivity in the transition-metal dichalcogenide PdTe₂ has been attributed to the proximity of a three-dimensional Van Hove singularity to the Fermi level. In isostructural NiTe₂, recently used as the weak link in a Josephson diode, a similar Van Hove singularity has been predicted to occur, but superconductivity is mysteriously absent. Using bulk-sensitive soft x-ray angle-resolved photoemission spectroscopy, we reveal that this Van Hove singularity lies even closer to the Fermi level in NiTe₂ than in PdTe₂. To explain the lack of superconductivity in NiTe₂, we perform *ab initio* calculations incorporating the Kukkonen Overhauser interaction, showing that an incipient magnetic instability suppresses superconductivity at an unprecedented scale. Finally, we present a tight-binding model that links the Van Hove singularity to a sign change in the Josephson diode effect at small magnetic fields, suggesting a new mechanism for Josephson diodes.

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The transition metal dichalcogenide NiTe₂ recently played an important role as a nonsuperconducting weak link between two superconducting niobium electrodes in a Josephson diode [1,2]. Studies of the surface electronic structure of NiTe₂ using angle-resolved photoelectron spectroscopy (ARPES) reveal spin-polarized topological surface states [1,3–6] that are believed to play a crucial role in the finite momentum Cooper pairing that induces the Josephson diode effect (JDE) in these junctions [1,7]. However, it is not clear if surface states alone can account for all the salient features of Josephson diodes. A sign change in the JDE observed at relatively low magnetic fields of 22 mT [1] would require very large effective g-factors if the JDE was only driven by surface states

shifted in energy by the Zeeman effect (see Sec. S1A of Supplemental Material [8]). Given the potential applications of Josephson diodes in future memory technologies [34], a comprehensive understanding of the electronic structure of materials underpinning the JDE is required.

While much is already known about the surface states in NiTe₂ [1,3–6] and previous works have detected bulk type-II Dirac nodes along the Γ -A momentum direction [3,4,35], little is known about bulk bands along other directions. In particular, there have been no investigations of a Van Hove singularity (VHs)—a saddle point in the band structure [Fig. 1(a)] [36]—at the M point in the three-dimensional (3D) bulk Brillouin zone [Fig. 1(b)]. Previously, this VHs was calculated to be ~ 100 – 150 meV below the Fermi level [4,6], but we instead calculate it to be 16 meV above E_F [Fig. 1(c)]. A similar 3D VHs was suggested to play an important role in the superconductivity of sister compound PdTe₂ [37]. Here, the electrons forming the VHs have been calculated to strongly couple to the Te phonon modes attributed to driving the superconductivity with an experimental $T_c = \sim 1.7$ K [38–40] [Fig. 1(d)]. A VHs with similarly strong coupling to phonon modes is predicted to appear in band structure calculations of NiTe₂ [5]. Properties of VHs bands and their effect on the DOS and electron-phonon coupling have also been linked to superconductivity and increased T_c in other materials [41–46].

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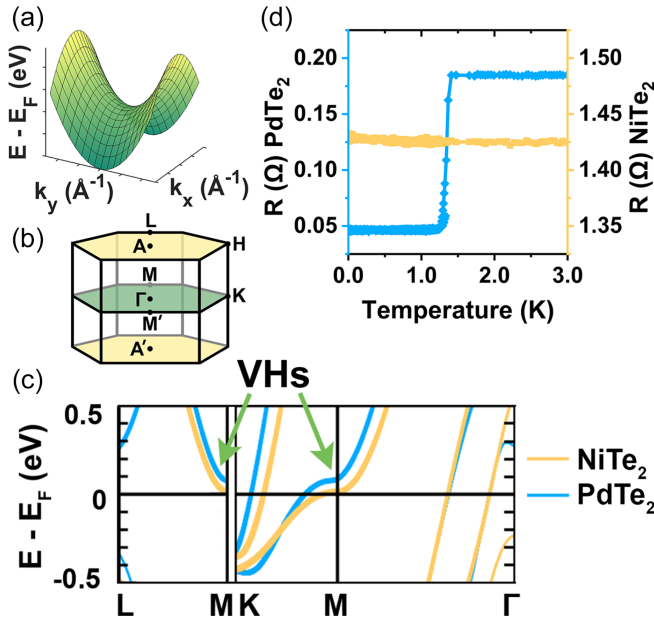


FIG. 1. (a) Saddle-point schematic showing the in-plane dispersion of a VHS. (b) Brillouin zone of NiTe_2 and PdTe_2 . (c) DFT band structure around the VHS (green arrows) in NiTe_2 and PdTe_2 . (d) Resistance curves measured for NiTe_2 and PdTe_2 . PdTe_2 resistance drops to zero at finite temperature as it becomes superconducting, whereas NiTe_2 remains resistive down to 8 mK. Zero offset in resistance arises from a calibration error.

Density functional theory (DFT) calculations suggest that the electronic and phononic [5] dispersions of NiTe_2 and PdTe_2 are extremely similar [Fig. 4(a)], which would suggest a similar superconducting transition temperature within traditional BCS-type superconductivity. Indeed, theoretical predictions by the Allen-Dynes formula suggest that NiTe_2 should have a finite T_c of 1.5 K [5] and 1.97 K in PdTe_2 [47]. However, superconductivity cannot be observed in bulk NiTe_2 even down to mK temperatures [Fig. 1(d)].

In this Letter, we use bulk sensitive soft x-ray ARPES to identify the precise location of the VHS in NiTe_2 and PdTe_2 . Single-crystal NiTe_2 and PdTe_2 samples were cleaved *in situ* at temperatures of ~ 14 K at the ADDRESS beamline [48,49] of the Swiss Light Source. Further details are provided in Sec. S2A of Supplemental Material [8]. Surprisingly, by fitting bands measured with ARPES we find the VHS pinned 16 meV above the Fermi level in nonsuperconducting NiTe_2 , but located 160 meV above E_F in superconducting PdTe_2 . To understand the puzzling absence of superconductivity in bulk NiTe_2 despite the favorable position of the VHS near E_F , we performed superconducting *ab initio* calculations that go beyond the random phase approximation (RPA) by including spin fluctuation effects. These calculations suggest that an incipient magnetic instability, absent in PdTe_2 , suppresses superconductivity in NiTe_2 at an unprecedented scale to less than 10% of its value obtained with conventional methods that do not include spin fluctuations. Additionally, we performed simulations with a phenomenological model

involving a magnetic field induced Lifshitz transition, which is known to occur for Van Hove singularities moving through E_F , to elucidate the role of the VHS in the JDE. Our model shows that even a very small magnetic-field-induced band shift can lead to a sign change in the JDE, suggesting that bulk electronic states could also contribute to the JDE observed in NiTe_2 -niobium Josephson junctions.

Experimental Fermi surfaces of NiTe_2 and PdTe_2 are shown in Figs. 2(a)–2(d) and contrasted with results from our DFT calculations [Figs. 2(e)–2(h)]. The green arrow in Figs. 2(a) and 2(b) indicates the position of the VHS in NiTe_2 , which can be identified by its characteristic “bowtie” shape in Fermi surfaces containing the M point, and is well reproduced by our calculations. In equivalent Fermi surfaces measured in PdTe_2 , there is no intensity at the M point suggesting the VHS is located further away from E_F . Note that not all expected features from the calculations can be observed in the experimental Fermi surfaces because of suppressed matrix elements in the photoemission process.

For further comparison to *ab initio* calculations and to extract the energy of the VHS, we show the experimentally measured dispersions along various high-symmetry directions in Fig. 3. The VHS along $L-M-\Gamma$, clear in NiTe_2 [green arrow in Fig. 3(a)] is notably absent in PdTe_2 [Fig. 3(c)]. This discrepancy suggests that E_{VHS} is above the Fermi level in PdTe_2 but very close to E_F in NiTe_2 . This is confirmed along the $\Gamma-K-M$ paths in Figs. 3(c) and 3(d) where the VHS band is almost exactly at the Fermi level in NiTe_2 , contrasted with a lack of spectral intensity at the M point in PdTe_2 . By fitting the VHS band, we determine that in NiTe_2 , $E_{VHS} = 16 \pm 20$ meV above E_F [Fig. 3(e)]. It is likely visible in the orthogonal spectrum along $\Gamma-M$ and $M-L$ [Fig. 3(a)] due to energy broadening across the Fermi level caused by the energy resolution of the experiment being 50–80 meV, electron-phonon coupling within a window of ~ 100 meV, or misalignment of the spectral cut in k_z (photon energy). In PdTe_2 , the VHS band is clearly above E_F and fitting the height of the VHS results in $E_{VHS} = 160 \pm 15$ meV [Fig. 3(f)].

From the correspondence of measured ARPES spectra to DFT calculations we can conclude that they describe the in-plane electronic structure of both NiTe_2 and PdTe_2 well. While they are less accurate in the out-of-plane direction, they still qualitatively describe the overall dispersive behaviors. Additionally, from the strong dependence of the dispersions on the out-of-plane momentum, we confirm the three-dimensional nature of the VHS.

For details on estimating E_{VHS} , see Sec. S2A of Supplemental Material [8]. Additional spectra are shown in Sec. S3 of Supplemental Material [8], alongside results of depositing elemental aluminum on the NiTe_2 surface to observe a possible doping-induced shift of the VHS, but where no identifiable change in E_{VHS} was observed. Additionally, Sec. S1C of Supplemental Material [8]

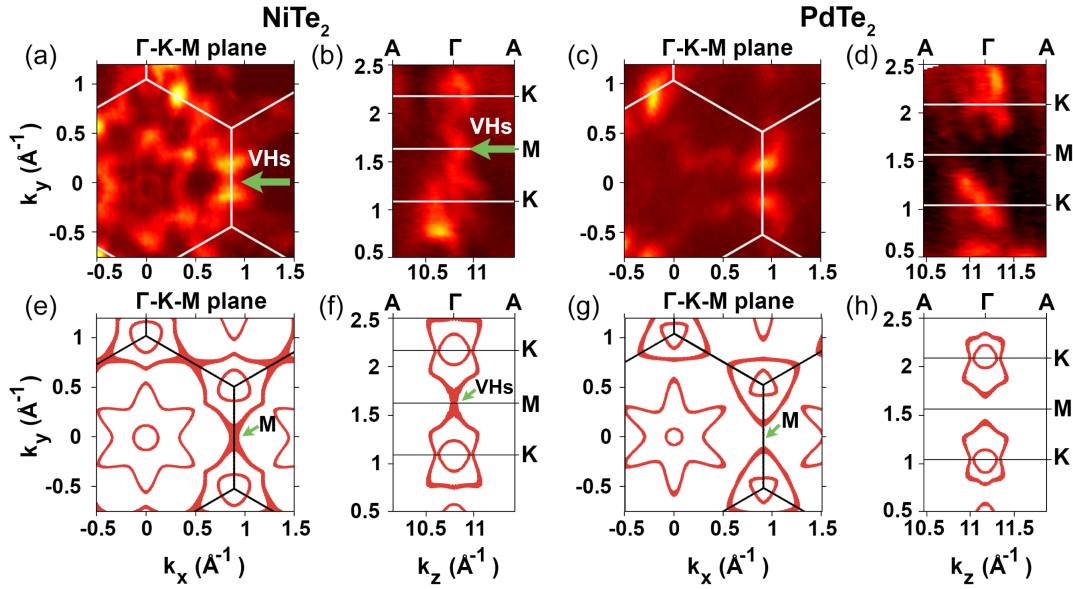


FIG. 2. Fermi surfaces of NiTe_2 and PdTe_2 . Green arrows point to a VHs at the M point. (a),(c) In-plane Fermi surface of NiTe_2 (PdTe_2) at the Γ -plane measured with ARPES with $h\nu = 535$ eV ($h\nu = 460$ eV) and s-polarization. (b),(d) Out-of-plane Fermi surface of NiTe_2 (PdTe_2) from a photon energy dependence. (e),(g) In-plane Fermi surface at the Γ -plane calculated with DFT broadened over a window of 25 meV in NiTe_2 and PdTe_2 . (f),(h) Out-of-plane Fermi surface DFT for NiTe_2 (PdTe_2).

discusses discrepancies between the NiTe_2 Γ -A DFT and ARPES results.

Our DFT calculations [Fig. 1(c)] place the VHs ~ 15 meV above the Fermi level in NiTe_2 and ~ 77 meV above E_F in PdTe_2 . We estimate an uncertainty of around 30 meV, arising from differences caused by using theoretically minimized lattice parameters versus experimental lattice parameters.

DFT simulations also suggest NiTe_2 has a density of states at E_F about 20% larger than in PdTe_2 , an important point for superconductivity [Fig. 4(b)]. A peak in the DOS of PdTe_2 corresponds to the position of the VHs at 160 meV. Based on this alone, and considering the overall similarity between these two systems, one could expect NiTe_2 to have a larger T_c than PdTe_2 . However, superconductivity in NiTe_2 was not observed.

To clarify this, we performed an *ab initio* characterization of these systems with a state-of-the-art method for conventional superconductivity. We computed the electron-phonon coupling using density functional perturbation theory and the superconducting state within fully *ab initio* superconducting density functional theory (SCDFT). Details of these calculations can be found in Sec. S2B of Supplemental Material [8]. We find that the electron-phonon coupling and T_c in NiTe_2 are indeed lower than in PdTe_2 , because the Pd compound has a slightly softer vibrational spectrum that in this low coupling regime is beneficial for superconductivity. Figure 4(a) shows the Eliashberg spectral function for NiTe_2 and PdTe_2 , the frequency dependence of the average electron-phonon coupling at E_F .

We find however, that the predicted critical temperatures are quite similar. We obtain $T_c^{\text{PdTe}_2} = 1.64$ K and $T_c^{\text{NiTe}_2} = 1.14$ K. $T_c^{\text{PdTe}_2}$ is extremely close to the experimental value of $T_c = \sim 1.7$ K. This raises the question of why superconductivity in NiTe_2 is not observed.

Our hypothesis is that the Ni compound may be close to an incipient magnetic instability, which can cause an enhancement of the spin susceptibility and spin fluctuation scattering in competition with the (already weak) electron-phonon coupling. This type of electronic pairing is neglected in conventional SCDFT simulations as these only account for the electronic charge response [50–52] by assuming an RPA screening. To test this possibility we resort to a recent development of the approach [53,54], which implements the Kukkonen Overhauser (KO) [55,56] interaction, effectively including both charge and spin density fluctuations. So far this method has been tested only on conventional superconductors where it has led to relatively small corrections in T_c , $\sim 20\%$ with respect to the RPA values [53,54,57]. Figure 4(c) compares the diagonal part of the Coulomb interaction $W(\epsilon, \epsilon)$ in NiTe_2 and PdTe_2 within the RPA and the KO approximation. The strength of the interaction in the two systems is comparable in RPA; however, when introducing spin fluctuation effects through the KO approximation, the Coulomb repulsion W in NiTe_2 becomes twice as strong as in PdTe_2 [see Fig. 4(c)].

The superconducting gap computed using both RPA and KO Coulomb interactions is shown in Fig. 4(d) as a function of the temperature. We find that including spin fluctuation effects in PdTe_2 reduces T_c to 1.38 K (16% compared to the RPA value); however, the same calculation

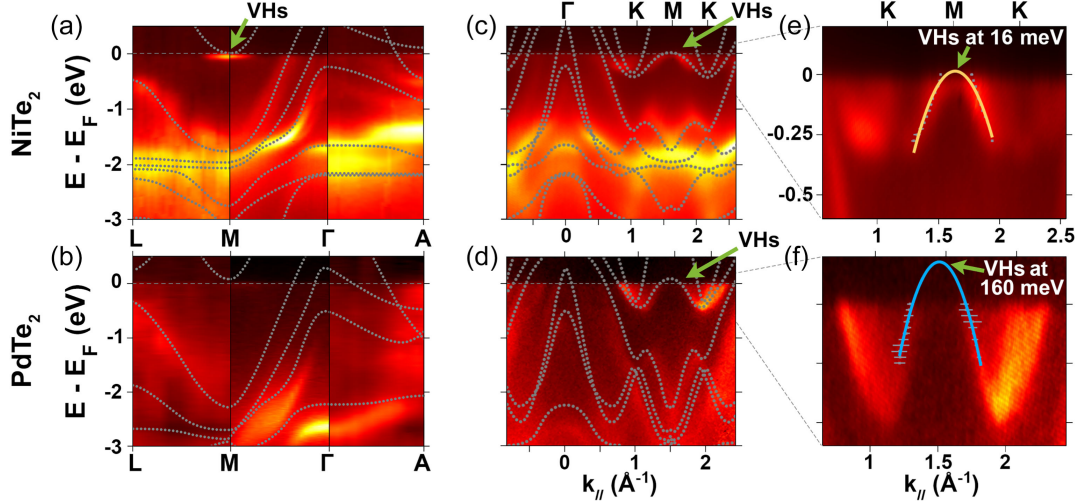


FIG. 3. Band structure of the VHS in NiTe₂ and PdTe₂ from ARPES. (a),(b) Spectral cuts through high-symmetry directions of NiTe₂ (PdTe₂) measured with s-polarization and photon energies between 400 and 550 eV. (c),(d) Spectral cut through Γ -K-M high-symmetry direction in NiTe₂(PdTe₂) showing VHS above E_F , measured with s-(p)-polarization and $h\nu = 535$ eV ($h\nu = 463$ eV). (e),(f) Close-up of (c),(d). We find the VHS is $16 \text{ meV} \pm 20 \text{ meV}$ ($160 \text{ meV} \pm 15 \text{ meV}$) above E_F .

for NiTe₂ leads to a negligible $T_c < 0.1$ K, consistent with experimental observations.

We have also investigated if it could be feasible to induce superconductivity in NiTe₂ by suppression of the magnetic instability via doping or pressure (see Sec. S1B of Supplemental Material [8]). It turns out that superconductivity is unlikely to occur below 5 GPa and below a hole doping level of the order of 1/4 electron per formula unit.

While it is not possible to extrapolate what calculations including the KO interaction will give for other materials without performing full-fledged simulations, it would be extremely interesting to explore the superconductivity of Kagome compounds that exhibit VHS and magnetic fluctuations in future work.

The development of a magnetic instability in NiTe₂, absent in PdTe₂, leads us to wonder if the VHS we observe near E_F still plays a role in the JDE in NiTe₂-niobium devices. As the VHS lies near the Fermi level, a magnetic field can induce a Lifshitz transition when the VHS passes through E_F , and we ask whether this change in topology could lead to the observed sign change in the JDE effect [1]. The asymmetry of the JDE may be traced to the multiple harmonics that are present in the current-phase relationship (CPR), $I_{JDE}(\phi) = I_1 \sin(\phi) + I_2 \sin(2\phi)$, where I_1 and I_2 represent the amplitudes of the first and second harmonic contributions, respectively. The sign of the JDE that is manifest depends directly on the relative signs of the harmonics. As in π -junctions, the change in the sign of I_c is by definition due to the change in sign of the first harmonic. In the specific context of the JDE, the correlation between the sign change in the JDE and the CPR has been established both experimentally [1,58] and theoretically [59,60].

To understand the quasiparticle dynamics close to a Lifshitz transition where the Fermi surface undergoes a change in topology, we constructed 3D tight-binding models including superconducting contacts and Rashba

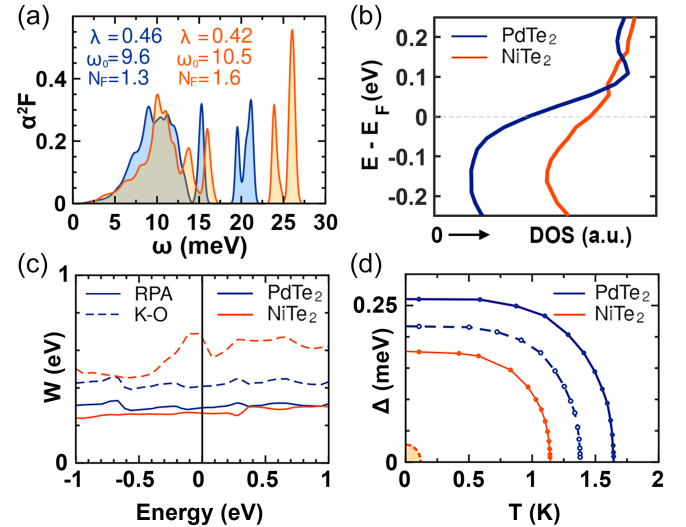


FIG. 4. *Ab initio* calculations. (a) Eliashberg spectral functions α^2F for bulk NiTe₂ (orange) and PdTe₂ (blue). λ is the electron-phonon coupling parameter, ω_0 is the logarithmic phonon average, and N_F is the density of states at the Fermi level in state per eV per cell. (b) Calculated DOS of NiTe₂ and PdTe₂. DOS at E_F is higher for NiTe₂. (c) Diagonal part of the effective Coulomb interaction $W(\epsilon, \epsilon)$ in the RPA (solid lines) and Kukkunen Overhauser (dashed lines) approximation (Sec. S2B of Supplemental Material [8]). (d) Superconducting gap Δ at the Fermi level as a function of temperature. The full area corresponding to NiTe₂ in the KO approximation indicates that the calculated T_c is less than 0.1 K.

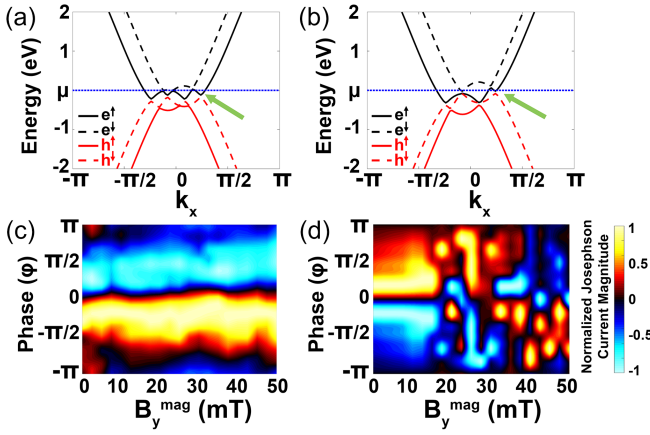


FIG. 5. Tight-binding model of the Josephson diode effect in the presence of a band inflection point. (a) Simulated electron (black) and hole (red) bands including spin-up (solid) and spin-down (dashed) contributions, showing the band inflection point similar to a VHS (green arrow) is below the chemical potential, μ . (b) The numerical band structure when μ is commensurate with E_F and the CPR switches sign; the band inflection point (green arrow) is calculated to be at the Fermi level. (c) The CPR as a function of the in-plane magnetic field when μ is not near the band inflection point. (d) The CPR when the band inflection point is near E_F . The current switches signs as the magnetic field causes the quantum critical point to pass through E_F .

spin-orbit coupling in the weak link, as well as the effect of an external magnetic field. Disorder effects and electron-phonon interactions are not included. When computing the Bogoliubov-de Gennes band structure of this material, we can see that near the Fermi level, a band inflection point appears [green arrows in Figs. 5(a) and 5(b)], similar to the saddle point of the Van Hove singularity that we observed in our ARPES measurements. Further model details with all used parameters are given in Sec. S2C of Supplemental Material [8], but it is important to note that we are using a moderate g -factor of 20 to include the effect of the magnetic field.

In Fig. 5(a) we plot the energy bands along the k_x momentum direction at $k_y = k_z = 0$ for $B_y = 0.05$ mT. We have chosen the chemical potential such that it is substantially above the band inflection point. As a result, when varying the magnetic field we observe no switching of the CPR, as shown in Fig. 5(c), meaning that the JDE effect will not change sign.

In Fig. 5(b), we plot the same one-dimensional band structure as in Fig. 5(a) but slightly shift the chemical potential 42 meV closer to the band inflection point and with $B_y = 0.20$ mT. With this inflection point being closer to the Fermi level, tuning the magnetic field will result in a switching of the CPR at a small magnetic field $B_y \approx 20$ mT [see Fig. 5(d)] as the magnetic field causes the band inflection point to pass through E_F , corresponding to a sign change of the JDE. At higher magnetic fields, the CPR undergoes several additional transitions.

On the level of this tight-binding model, we can conclude that a magnetic-field-induced Lifshitz transition in a model with a band inflection point near E_F in the weak link can indeed lead to the experimentally observed sign change in the JDE at relatively low magnetic fields using moderate g -factors. While this theoretical model suggests a new mechanism for the Josephson diode effect, detailed quantitative theoretical modeling with realistic material parameters is left for future studies.

An important open question is the relative role of bulk versus surface states in the JDE. A promising reference system is 1T-PtSe₂, which hosts Van Hove singularities but no topological surface states [61]. Future ARPES and JDE studies on Nb-PtSe₂ could therefore help disentangle bulk and interface contributions.

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Data availability—The data that support the findings of this article are openly available [62].

- [1] B. Pal, A. Chakraborty, P. K. Sivakumar, M. Davydova, A. K. Gopi, A. K. Pandeya, J. A. Krieger, Y. Zhang, M. Date, S. Ju, N. Yuan, N. B. M. Schröter, L. Fu, and S. S. P. Parkin, Josephson diode effect from Cooper pair momentum in a topological semimetal, *Nat. Phys.* **18**, 1228 (2022).
- [2] V. D. Esin, O. O. Shvetsov, A. V. Timonina, N. N. Kolesnikov, and E. V. Deviatov, Interface superconductivity in a Dirac semimetal NiTe₂, *Nanomater. Nanotechnol.* **12**, 4114 (2022).
- [3] B. Ghosh, D. Mondal, C.-N. Kuo, C. S. Lue, J. Nayak, J. Fujii, I. Vobornik, A. Politano, and A. Agarwal, Observation of bulk states and spin-polarized topological surface states in transition metal dichalcogenide Dirac semimetal candidate NiTe₂, *Phys. Rev. B* **100**, 195134 (2019).
- [4] S. Mukherjee, S. W. Jung, S. F. Weber, C. Xu, D. Qian, X. Xu, P. K. Biswas, T. K. Kim, L. C. Chapon, M. D. Watson, J. B. Neaton, and C. Cacho, Fermi-crossing Type-II Dirac fermions and topological surface states in NiTe₂, *Sci. Rep.* **10**, 12957 (2020).

- [5] J. Zhang and G. Q. Huang, The superconductivity and topological surface state of type-II Dirac semimetal NiTe_2 , *J. Phys. Condens. Matter* **32**, 205702 (2020).
- [6] C. Xu, B. Li, W. Jiao, W. Zhou, B. Qian, R. Sankar, N. D. Zhigadlo, Y. Qi, D. Qian, F.-C. Chou, and X. Xu, Topological type-II Dirac fermions approaching the Fermi level in a transition metal dichalcogenide NiTe_2 , *Chem. Mater.* **30**, 4823 (2018).
- [7] A. Q. Chen, M. J. Park, S. T. Gill, Y. Xiao, D. Reig-i Plessis, G. J. MacDougall, M. J. Gilbert, and N. Mason, Finite momentum Cooper pairing in three-dimensional topological insulator Josephson junctions, *Nat. Commun.* **9**, 3478 (2018).
- [8] See Supplemental Material at <http://link.aps.org/supplemental/10.1103/hp1t-zd7y>, which includes Refs. [9–33] for which contains additional calculations; technical details on the experimental procedure, data analysis and calculations contained in the main text; and additional ARPES data.
- [9] Z. Feng, J. Si, T. Li, H. Dong, C. Xu, J. Yang, Z. Zhang, K. Wang, H. Wu, Q. Hou, J. J. Xing, S. Wan, S. Li, W. Deng, J. Feng, A. Pal, F. Chen, S. Hu, J. Y. Ge, C. Dong, S. Wang, W. Ren, S. Cao, Y. Liu, X. Xu, J. Zhang, B. Chen, and N. C. Yeh, Evidences for pressure-induced two-phase superconductivity and mixed structures of NiTe_2 and NiTe in type-II Dirac semimetal NiTe_{2-x} ($x = 0.38 \pm 0.09$) single crystals, *Mater. Today Phys.* **17**, 100339 (2021).
- [10] B. de Lima, R. de Cassia, F. Santos, L. Correa, T. Grant, A. Manesco, G. Martins, L. Eleno, M. Torikachvili, and A. Machado, Properties and superconductivity in Ti-doped NiTe_2 single crystals, *Solid State Commun.* **283**, 27 (2018).
- [11] R. Queiroz, G. Landolt, S. Muff, B. Slomski, T. Schmitt, V. N. Strocov, J. Mi, B. B. Iversen, P. Hofmann, J. Osterwalder, A. P. Schnyder, and J. H. Dil, Sputtering-induced reemergence of the topological surface state in Bi_2Se_3 , *Phys. Rev. B* **93**, 165409 (2016).
- [12] A. Tkatchenko and M. Scheffler, Accurate molecular van der Waals interactions from ground-state electron density and free-atom reference data, *Phys. Rev. Lett.* **102**, 073005 (2009).
- [13] M. Dion, H. Rydberg, E. Schröder, D. C. Langreth, and B. I. Lundqvist, Van der Waals density functional for general geometries, *Phys. Rev. Lett.* **92**, 246401 (2004).
- [14] G. Román-Pérez and J. M. Soler, Efficient implementation of a van der Waals density functional: Application to double-wall carbon nanotubes, *Phys. Rev. Lett.* **103**, 096102 (2009).
- [15] HQGraphene, <https://www.hqgraphene.com/>.
- [16] MATools ARPES data analysis package, Available from <https://drive.switch.ch/index.php/s/jiaxJHX14jFbQ83>.
- [17] P. Hohenberg and W. Kohn, Inhomogeneous electron gas, *Phys. Rev.* **136**, B864 (1964).
- [18] W. Kohn and L. J. Sham, Self-consistent equations including exchange and correlation effects, *Phys. Rev.* **140**, A1133 (1965).
- [19] J. P. Perdew, A. Ruzsinszky, G. I. Csonka, O. A. Vydrov, G. E. Scuseria, L. A. Constantin, X. Zhou, and K. Burke, Restoring the density-gradient expansion for exchange in solids and surfaces, *Phys. Rev. Lett.* **100**, 136406 (2008).
- [20] The Elk FP-LAPW Code, <http://elk.sourceforge.net/>.
- [21] S. Baroni, P. Giannozzi, and A. Testa, Green's-function approach to linear response in solids, *Phys. Rev. Lett.* **58**, 1861 (1987).
- [22] P. Giannozzi *et al.*, Quantum Espresso: A modular and open-source software project for quantum simulations of materials, *J. Phys. Condens. Matter* **21**, 395502 (2009).
- [23] P. Giannozzi *et al.*, Advanced capabilities for materials modelling with Quantum Espresso, *J. Phys. Condens. Matter* **29**, 465901 (2017).
- [24] M. van Setten, M. Giantomassi, E. Bousquet, M. Verstraete, D. Hamann, X. Gonze, and G.-M. Rignanese, The PseudoDojo: Training and grading a 85 element optimized norm-conserving pseudopotential table, *Comput. Phys. Commun.* **226**, 39 (2018).
- [25] L. N. Oliveira, E. K. U. Gross, and W. Kohn, Density-functional theory for superconductors, *Phys. Rev. Lett.* **60**, 2430 (1988).
- [26] M. Lüders, M. A. L. Marques, N. N. Lathiotakis, A. Floris, G. Profeta, L. Fast, A. Continenza, S. Massidda, and E. K. U. Gross, Ab initio theory of superconductivity. I. Density functional formalism and approximate functionals, *Phys. Rev. B* **72**, 024545 (2005).
- [27] A. Sanna, C. Pellegrini, and E. K. U. Gross, Combining Eliashberg theory with density functional theory for the accurate prediction of superconducting transition temperatures and gap functions, *Phys. Rev. Lett.* **125**, 057001 (2020).
- [28] J. P. Perdew and A. Zunger, Self-interaction correction to density-functional approximations for many-electron systems, *Phys. Rev. B* **23**, 5048 (1981).
- [29] P. B. Allen and B. Mitrović, Theory of Superconducting T_c , *Solid State Physics* Vol. 37 (Academic Press, New York, 1983), pp. 1–92.
- [30] J. A. Flores-Livas, L. Boeri, A. Sanna, G. Profeta, R. Arita, and M. Eremets, A perspective on conventional high-temperature superconductors at high pressure: Methods and materials, *Phys. Rep.* **856**, 1 (2020).
- [31] A. Sanna, C. Pellegrini, E. Liebhaber, K. Rossnagel, K. J. Franke, and E. K. U. Gross, Real-space anisotropy of the superconducting gap in the charge-density wave material 2H-NbSe_2 , *npj Quantum Mater.* **7**, 6 (2022).
- [32] R. Lake, G. Klimeck, R. C. Bowen, and D. Jovanovic, Single and multiband modeling of quantum electron transport through layered semiconductor devices, *J. Appl. Phys.* **81**, 7845 (1997).
- [33] Q.-f. Sun, J. Wang, and T.-h. Lin, Control of the supercurrent in a mesoscopic four-terminal Josephson junction, *Phys. Rev. B* **62**, 648 (2000).
- [34] R. Hess, H. F. Legg, D. Loss, and J. Klinovaja, Josephson transistor from the superconducting diode effect in domain wall and skyrmion magnetic racetracks, *Phys. Rev. B* **108**, 174516 (2023).
- [35] M. Nurmamat, S. V. Eremeev, X. Wang, T. Yoshikawa, T. Kono, M. Kakoki, T. Muro, Q. Jiang, Z. Sun, M. Ye, and A. Kimura, Bulk Dirac cone and highly anisotropic electronic structure of NiTe_2 , *Phys. Rev. B* **104**, 155133 (2021).
- [36] W. Wu, Z. Shi, M. Ozerov, Y. Du, Y. Wang, X.-S. Ni, X. Meng, X. Jiang, G. Wang, C. Hao, X. Wang, P. Zhang, C. Pan, H. Pan, Z. Sun, R. Yang, Y. Xu, Y. Hou, Z. Yan, C. Zhang, H.-Z. Lu, J. Chu, and X. Yuan, The discovery of

- three-dimensional Van Hove singularity, *Nat. Commun.* **15**, 2313 (2024).
- [37] K. Kim, S. Kim, J. S. Kim, H. Kim, J.-H. Park, and B. I. Min, Importance of the Van Hove singularity in superconducting PdTe₂, *Phys. Rev. B* **97**, 165102 (2018).
- [38] H. Leng, C. Paulsen, Y. K. Huang, and A. De Visser, Type-I superconductivity in the Dirac semimetal PdTe₂, *Phys. Rev. B* **96**, 220506 (2017).
- [39] Amit and Y. Singh, Heat capacity evidence for conventional superconductivity in the type-II Dirac semimetal PdTe₂, *Phys. Rev. B* **97**, 054515 (2018).
- [40] S. Das, Amit, A. Sirohi, L. Yadav, S. Gayen, Y. Singh, and G. Sheet, Conventional superconductivity in the type-II Dirac semimetal PdTe₂, *Phys. Rev. B* **97**, 014523 (2018).
- [41] Y. Hu, X. Wu, B. R. Ortiz, S. Ju, X. Han, J. Ma, N. C. Plumb, M. Radovic, R. Thomale, S. D. Wilson, A. P. Schnyder, and M. Shi, Rich nature of Van Hove singularities in Kagome superconductor CsV₃Sb₅, *Nat. Commun.* **13**, 2220 (2022).
- [42] M. Kang, S. Fang, J.-K. Kim, B. R. Ortiz, S. H. Ryu, J. Kim, J. Yoo, G. Sangiovanni, D. Di Sante, B.-G. Park, C. Jozwiak, A. Bostwick, E. Rotenberg, E. Kaxiras, S. D. Wilson, J.-H. Park, and R. Comin, Twofold van Hove singularity and origin of charge order in topological kagome superconductor CsV₃Sb₅, *Nat. Phys.* **18**, 301 (2022).
- [43] W. Sano, T. Koretsune, T. Tadano, R. Akashi, and R. Arita, Effect of Van Hove singularities on high- T_c superconductivity in H₃S, *Phys. Rev. B* **93**, 094525 (2016).
- [44] Y. Quan and W. E. Pickett, Van Hove singularities and spectral smearing in high-temperature superconducting H₃S, *Phys. Rev. B* **93**, 104526 (2016).
- [45] H. Yao and F. Yang, Topological odd-parity superconductivity at type-II two-dimensional van Hove singularities, *Phys. Rev. B* **92**, 035132 (2015).
- [46] T.-T. Gai, P.-J. Guo, H.-C. Yang, Y. Gao, M. Gao, and Z.-Y. Lu, Van Hove singularity induced phonon-mediated superconductivity above 77 K in hole-doped SrB₃C₃, *Phys. Rev. B* **105**, 224514 (2022).
- [47] R. C. Xiao, P. L. Gong, Q. S. Wu, W. J. Lu, M. J. Wei, J. Y. Li, H. Y. Lv, X. Luo, P. Tong, X. B. Zhu, and Y. P. Sun, Manipulation of type-I and type-II Dirac points in PdTe₂ superconductor by external pressure, *Phys. Rev. B* **96**, 075101 (2017).
- [48] V. N. Strocov, X. Wang, M. Shi, M. Kobayashi, J. Krempasky, C. Hess, T. Schmitt, and L. Patthey, Soft-x-ray ARPES facility at the ADRESS beamline of the SLS: Concepts, technical realisation and scientific applications, *J. Synchrotron Radiat.* **21**, 32 (2014).
- [49] V. N. Strocov, T. Schmitt, U. Flechsig, T. Schmidt, A. Imhof, Q. Chen, J. Raabe, R. Betemps, D. Zimoch, J. Krempasky, X. Wang, M. Grioni, A. Piazzalunga, and L. Patthey, High-resolution soft x-ray beamline ADRESS at the Swiss Light Source for resonant inelastic x-ray scattering and angle-resolved photoelectron spectroscopies, *J. Synchrotron Radiat.* **17**, 631 (2010).
- [50] M. A. L. Marques, M. Lüders, N. N. Lathiotakis, G. Profeta, A. Floris, L. Fast, A. Continenza, E. K. U. Gross, and S. Massidda, Ab initio theory of superconductivity. II. Application to elemental metals, *Phys. Rev. B* **72**, 024546 (2005).
- [51] S. Massidda, F. Bernardini, C. Bersier, A. Continenza, P. Cudazzo, A. Floris, H. Glawe, M. Monni, S. Pittalis, G. Profeta, A. Sanna, S. Sharma, and E. K. U. Gross, The role of Coulomb interaction in the superconducting properties of CaC₆ and H under pressure, *Supercond. Sci. Technol.* **22**, 034006 (2009).
- [52] A. Sanna, G. Profeta, A. Floris, A. Marini, E. K. U. Gross, and S. Massidda, Anisotropic gap of superconducting CaC₆: A first-principles density functional calculation, *Phys. Rev. B* **75**, 020511(R) (2007).
- [53] C. Pellegrini, C. Kukkonen, and S. Antonio, Ab initio calculations of superconducting transition temperatures: When going beyond RPA is essential, *Phys. Rev. B* **108**, 064511 (2023).
- [54] C. Pellegrini and A. Sanna, Ab initio methods for superconductivity, *Nat. Rev. Phys.* **6**, 509 (2024).
- [55] C. A. Kukkonen and A. W. Overhauser, Electron-electron interaction in simple metals, *Phys. Rev. B* **20**, 550 (1979).
- [56] G. Vignale and K. S. Singwi, Effective two-body interaction in Coulomb Fermi liquids, *Phys. Rev. B* **32**, 2156 (1985).
- [57] A. Cucciarri, D. Naddeo, S. Di Cataldo, and L. Boeri, NbTi: A nontrivial puzzle for the conventional theory of superconductivity, *Phys. Rev. B* **110**, L140502 (2024).
- [58] C. Baumgartner, L. Fuchs, A. Costa, S. Reinhardt, S. Gronin, G. C. Gardner, T. Lindemann, M. J. Manfra, P. E. Faria Junior, D. Kochan, J. Fabian, N. Paradiso, and C. Strunk, Supercurrent rectification and magnetochiral effects in symmetric Josephson junctions, *Nat. Nanotechnol.* **17**, 39 (2022).
- [59] R. S. Souto, M. Leijnse, and C. Schrade, Josephson diode effect in supercurrent interferometers, *Phys. Rev. Lett.* **129**, 267702 (2022).
- [60] M. Davydova, S. Prembabu, and L. Fu, Universal Josephson diode effect, *Sci. Adv.* **8**, eabo0309 (2022).
- [61] O. Clark, M. Neat, K. Okawa, L. Bawden, I. Marković, F. Mazzola, J. Feng, V. Sunko, J. Riley, W. Meevasana, J. Fujii, I. Vobornik, T. Kim, M. Hoesch, T. Sasagawa, P. Wahl, M. Bahramy, and P. King, Fermiology and superconductivity of topological surface states in PdTe₂, *Phys. Rev. Lett.* **120**, 156401 (2018).
- [62] McFarlane *et al.*, Van Hove singularities, superconductivity, and the Josephson diode effect in NiTe₂ and PdTe₂, Available at, [10.17617/3.2PXLY6](https://arxiv.org/abs/10.17617/3.2PXLY6) (Edmond 2026).