Single-layer $\beta$-Bi$_2$Pd: a phonon-mediated 2D topological superconductor

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Topological superconductors, characterized by topologically nontrivial states residing in a superconducting gap, are a recently discovered class of materials having Majorana Fermions. Several single-material 3D topological superconductors have been theoretically predicted and experimentally confirmed. Here, we show that 2D single-layer $\beta$-Bi$_2$Pd, is an intrinsic electron-phonon superconductor with nontrivial Fu-Kane $Z_2$ indices and topological edge states. This then leads to the expectation of 2D topological superconductivity and Majorana bound states in monolayer $\beta$-Bi$_2$Pd.

I. INTRODUCTION

Two dimensional (2D) superconductors, while known, as in Pb thin films1–4, have attracted much recent interest due to discoveries such as evidence for very high critical temperatures in oxide supported monolayer FeSe5,6, the superconductivity of bilayer twisted graphene7, the finding of unconventional behavior in strong spin orbit split cases8 and the finding of undiminished high temperature superconductivity in cuprate monolayers9. Furthermore, 2D materials enable unique device geometries due to the ability to fabricate stacked structures and manipulate properties. A particular interest is in devices related to quantum information. In this regard, superconductors with nontrivial topological states are of interest due to the possibility of achieving Majorana Fermions10,11.

There have been a number of reports observing superconductivity in topologically nontrivial systems with signatures of unusual superconductivity. These include Cu or Sr-doped Bi$_2$Se$_3$12–15, Bi$_2$Se$_3$/NbSe$_2$ heterostructures16,17, Bi$_2$Te$_3$ or Bi$_2$Te on Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$18, atomic Fe chains on Pb(110)19, and Nb structures on (C$_{6}$,12 Bi$_{0.26}$Sb$_{0.62}$)$_2$Te$_3$ thin films20. These generally involve production of superconductivity by doping topological materials or by proximity effects. While these are effective strategies18,19, it is desirable to identify intrinsic topological superconductors, particularly with chemical stoichiometry20–25, as well as 2D versions.

Evidence for Majorana zero modes was found in some intrinsic 3D superconductors such as 2M phase WS$_2$26,27, $T_d$-MoTe$_2$28, BiPd29, $\beta$-Bi$_2$Pd, and PbTaSe$_2$30. Of these $\beta$-Bi$_2$Pd is of particular interest due to its naturally layered crystal structure[see Fig. 1(a)], which suggests the possibility of realizing a 2D topological superconductor. Layered $\beta$-Bi$_2$Pd is a superconductor with a full superconducting gap31. The compound is centrosymmetric (space group I4/mmm) with superconducting critical temperature, $T_c=5.4$ K32. Furthermore, the compound has nontrivial band topology33. This makes it a promising candidate for investigation of bulk topological superconductivity, independent of doping or proximity effects34. The crystal structure is composed of Bi$_2$Pd sheets, consisting of Pd atoms between Bi planes35–37. This suggests the possibility of forming monolayers, since it may be expected that Bi-Bi bonding between the Bi$_2$Pd sheets will be weak. In fact, the material is amenable to thin film growth, and it is found that such films are superconducting with evidence for topological behavior36.

Here we use first principles calculations to show that single-layer $\beta$-Bi$_2$Pd is a 2D electron phonon superconductor, and that it has a topological electronic structure based on the $Z_2$ invariant. Specifically, we start with the layered structure and present a theoretical study of the electronic structure, topological properties, and superconductivity of single-layer $\beta$-Bi$_2$Pd via state-of-the-art first-principles calculations. We find that it has nontrivial topology and the $Z_2$ topological invariant38,39. Single-layer $\beta$-Bi$_2$Pd has a two-band Fermi surface with mixed Bi-p/Pd-d orbital character. Detailed calculations of the electron phonon Eliashberg spectral function, $\omega^2 F(\omega)$ show that electron phonon superconductivity is present. Strong contributions are found both for optic phonons that intersect the acoustic branches with strong Bi contributions, as well as higher frequency modes with Pd character. Taking together the superconductivity and nontrivial topological states of single-layer $\beta$-Bi$_2$Pd, our work points out a real material that is a promising platform for studying topological superconductivity and Majorana physics in the 2D limit.

II. COMPUTATIONAL METHODS

Our calculations were performed within density functional theory with norm-conserving pseudopotentials40,41 as implemented in the Quantum-ESPRESSO package42,43. We used the Perdew–Burke–Ernzerhof44,45 generalized gradient approximation. All self-consistent calculations were performed with a planewave kinetic energy cutoff of 80 Ry. We used a Brillouin zone (BZ) sampling based on a $32 \times 32 \times 1$ $k$-mesh. A
Methfessel-Paxton smearing of 0.02 Ry was employed for these calculations. The internal atomic positions were fully relaxed with a threshold of 10 meV/Å for the forces. We did calculations using a supercell, of length 15 Å along the z direction.

The phonon spectrum and electron-phonon coupling (EPC) strength \( \lambda \) were calculated with density functional perturbation theory on a \( 8 \times 8 \times 1 \) \( q \)-mesh. Here, the mode-resolved magnitude of the EPC \( \lambda_{q\nu} \) is calculated according to the Migdal-Eliashberg theory \(^{46,47}\) by

\[
\lambda_{q\nu} = \frac{\gamma_{q\nu}}{\hbar N(E_F)\omega_{q\nu}^2},
\]

(1)

where \( \gamma_{q\nu} \) is the phonon linewidth, \( \omega_{q\nu} \) is the phonon frequency, and \( N(E_F) \) is the electronic density of states at the Fermi level. The \( \gamma_{q\nu} \) can be obtained with

\[
\gamma_{q\nu} = \frac{2\pi\omega_{q\nu}}{\Omega_{BZ}} \sum_{k,n,m} |g_{k\nu,k+q,n,m}|^2 \delta(\varepsilon_{nk} - E_F)\delta(\varepsilon_{k+qn,m} - E_F),
\]

(2)

where \( \Omega_{BZ} \) is the volume of BZ, \( \varepsilon_{nk} \) and \( \varepsilon_{k+qn,m} \) denote the Kohn-Sham energy, and \( g_{k\nu,k+q,n,m} \) is the EPC matrix element. The \( g_{k\nu,k+q,n,m} \), which can be determined self-consistently by the linear response theory, describe the probability amplitude for the scattering of an electron with a transfer of crystal momentum \( q \).\(^{48}\) The Eliashberg electron-phonon spectral function \( \alpha^2 F(\omega) \) is then

\[
\alpha^2 F(\omega) = \frac{1}{2\pi N(E_F)} \sum_{q\nu} \frac{\gamma_{q\nu}}{\omega_{q\nu}} \delta(\omega - \omega_{q\nu}).
\]

(3)

The EPC constant \( \lambda \) can be calculated either by the summation of the EPC constant \( \lambda_{q\nu} \) in the full BZ for all phonon modes or by the integral of the Eliashberg spectral function \( \alpha^2 F(\omega) \)\(^{49}\) as

\[
\lambda(\omega) = \sum_{q\nu} \lambda_{q\nu} = 2 \int_0^\infty \frac{\alpha^2 F(\omega)}{\omega} d\omega.
\]

(4)

We use the McMillan-Allen-Dynes formula to obtain the superconducting transition temperature, \( T_c \), from the calculated EPC constant \( \lambda \),

\[
T_c = f_1 f_2 \frac{\omega_{\text{log}}}{1.2} \exp \left[ -\frac{1.04(1 + \lambda)}{\lambda - \mu^*(1 + 0.62\lambda)} \right],
\]

(5)

where \( \mu^* \) is the effective screened Coulomb repulsion constant, \( \omega_{\text{log}} \) is the logarithmic average frequency,

\[
\omega_{\text{log}} = \exp \left[ \frac{2}{A} \int_0^\infty \frac{d\omega}{\omega} \alpha^2 F(\omega) \log \omega \right],
\]

(6)

and \( f_1 \) is the correction factor when \( \lambda > 1.350 \). In our calculation, \( \mu^* = 0.1 \) and \( f_1 f_2 = 1 \) were used. This is based on parameters used in bulk \( \beta\)-Bi\(_2\)-Pd previously\(^{51}\).

In order to analyze the topology and specifically establish the presence of edge states, we used a tight binding Hamiltonian, constructed from the first-principles Bloch functions. This was done by projecting Bloch states onto maximally localized Wannier functions (MLWFs)\(^{52}\) with the Wannier90 package\(^{53,54}\). In the model, the MLWFs are derived from atomic Bi-s, Bi-p, and Pd-d orbitals. Using the MLWFs, the edge states are calculated from the imaginary part of the surface Green’s function\(^{55}\) as provided by the WannierTools package\(^{56}\).

III. RESULTS AND DISCUSSION

A. Crystal and band structures

![FIG. 1. (a) Side view of bulk \( \beta\)-Bi\(_2\)-Pd crystal. (b) Side and (c) top views of single-layer \( \beta\)-Bi\(_2\)-Pd. The purple and gray balls indicate Bi and Pd atoms, respectively. Unit cells are indicated by the solid black line.](image-url)

As mentioned, \( \beta\)-Bi\(_2\)-Pd is a layered compound with tetragonal centrosymmetric space group, \( I4/mmm \), with Bi on site 4e and Pd on 2a, as shown in Fig. 1(a)\(^{34–37}\). The structure can be described as a close packed stacking of triple layers each consisting of a square Pd atomic layer sandwiched between two square Bi atomic layers to yield layering sequence, Bi-Pd-Bi. As discussed in prior work, the bonding within a triple layer, particularly the Pd-Bi bonding is substantially stronger than the Bi-Bi bonding between different triple layer units\(^{34}\). Thus monolayers consisting of triple layer sheets can be made using molecular beam epitaxy\(^{37}\), similar to many 2D metal chalcogenides and related materials\(^{58}\).

We construct the monolayer compound starting with the bulk structure. The primitive cell of monolayer \( \beta\)-Bi\(_2\)-Pd is square with two Bi and one Pd atoms in one unit. The optimized lattice constant is calculated to be 3.352 Å, which is slightly smaller than the experimental lattice constant (3.362 Å) of bulk \( \beta\)-Bi\(_2\)-Pd\(^{51}\). The Bi-Pd bond length is stretched to 2.999 Å compared with measured bulk value. This leads to a monolayer thickness measured from Bi in the top layer to Bi in the bottom layer of 3.674 Å.

The electronic structure near the Fermi level is metallic and is derived from hybridized bands of primarily Bi p and Pd d character. The Bi p states in particular are subject to strong...
Effects of spin orbit coupling (SOC). Figures 2(a-b) depict the orbital projected band structure of single-layer $\beta$-Bi$_2$Pd along the main high-symmetry directions of the BZ without the inclusion of SOC. The band structure without SOC clearly shows the valence band and conduction band touch at the M point and along the $\Gamma$-M line. Two bands cross the Fermi level leading to the metallic nature. SOC leads to splitting of degenerate bands around the Fermi level in Figs. 2(c-d). Importantly, the bands crossing the Fermi level are gapped from each other, so that there is a continuous gap between them over the whole BZ. This full-gap feature, which is important for producing a topological superconductor, also appears in bulk $\beta$-Bi$_2$Pd, Au$_2$Pd, and PbTaSe$_2$, as shown by first-principles calculations and experimental measurements. In the present case, the gapping is large, reflecting the strong effect of SOC on Bi p orbitals.

**TABLE I.** The parities of occupied bands below the full gap at $\Gamma$, X, Y, and M points in the BZ for single-layer $\beta$-Bi$_2$Pd. There are 40 electrons in one unit cell, corresponding to 20 occupied bands with SOC for this centrosymmetric structure. The products of the parities of the Bloch wave functions for the occupied energy bands at the four time-reversal-invariant-momenta (TRIM) points, respectively, which yields a nontrivial topological invariant $\nu = 1$ for single-layer $\beta$-Bi$_2$Pd.

| TRIMs | Parities of occupied spin-degenerate bands | Product |
|-------|---------------------------------|---------|
| $\Gamma$ | - + + - + - + - - + + + + + + + + + - - | - |
| X, Y | - + + - + - + - + - + + + + + + + + + + + | + |
| M | + - + - + - + - + + - + + - + + + + + + | + |

Monolayer $\beta$-Bi$_2$Pd having point group $D_{4h}$, is centrosymmetric and as mentioned has a full energy gap throughout the whole BZ. Because of this, parity analysis can be used to compute the $Z_2$ invariant ($\nu$). This enables classification into a topologically nontrivial phase of $\nu = 1$ or a topologically trivial phase of $\nu = 0$ for the system. According to the Fu-Kane method, the $Z_2$ topological invariant comes from the parities of the Bloch wave functions for the occupied energy bands. Table I shows the parities of twenty occupied bands at $\Gamma$, X, Y, and M, respectively. For monolayer $\beta$-Bi$_2$Pd, the products of the parity eigenvalues at $\Gamma$, X, Y, and M points are -1, +1, +1, and +1, respectively. This makes the system topologically nontrivial with $\nu = 1$.

Typically, nontrivial topology of a two-dimensional material (such as graphene) guarantees the existence of gapless edge states at its one-dimensional boundary. These are a direct consequence of the nontrivial topology. We performed edge-state calculations by the Greens-function approach for the corresponding semi-infinite systems to explicitly verify this for monolayer $\beta$-Bi$_2$Pd. The calculated results for monolayer $\beta$-Bi$_2$Pd with SOC, presented in Figs. 3(a) and 3(b) show that one gapless edge state connects the valence and conduction bands at X point for Bi-terminated and Pd-terminated ribbons, respectively. There are also additional edge states in Fig. 3, owing to the existence of Dirac points in the band structure of Fig. 2. With SOC, the split bulk states harbor topological Dirac-like states lying in the continuous energy gap around the X point [Figs. 3(c) and 3(d)]. This confirms the bulk-boundary correspondence between the bulk topological invariants and the surface-state configurations, demonstrating that single-layer $\beta$-Bi$_2$Pd indeed hosts nontrivial topology.

**TABLE II.** $N(E_F)$ (in unit of states per spin per eV per cell), $\omega_{\log}$ (in K), $\lambda$, and $T_c$ (in K) for $\beta$-Bi$_2$Pd. The values in parentheses are calculated with SOC.

| Comp. | $N(E_F)$ | $\omega_{\log}$ | $\lambda$ | $T_c$ | Ref. |
|-------|----------|----------------|----------|------|------|
| 2D    | 0.66     | 73.93         | 0.63     | 1.95 | Ours |
| 3D    | 0.66 (0.79) | 101.72 (68.53) | 0.77 (0.97) | 4.40 (4.55) | 51  |
| 3D    | 1.331    | 83.89         | 0.81     | 4.04 | 63   |

**C. Phonons and electron phonon superconductivity**


FIG. 3. Calculated topological edge states of single-layer $\beta$-Bi$_2$Pd for (a) Bi-terminated and (b) Pd-terminated ribbons. Panels (c)-(d) are the same as panels (a)-(b), respectively, but with SOC. The Fermi level is set to zero. The edge states connect the bulk valence and conduction bands.

FIG. 4. (a) Calculated phonon dispersion along high symmetry lines for monolayer $\beta$-Bi$_2$Pd. The size of red circles is proportional to the magnitude of $\lambda_{qm}$. (b) Projected phonon density of states for single-layer $\beta$-Bi$_2$Pd. (c) Frequency-dependent Eliashberg spectral function $\alpha^2 F(\omega)$ and cumulative frequency-dependent EPC function $\lambda(\omega)$ for single-layer $\beta$-Bi$_2$Pd. The black dots in the panel (c) are at 30, 42, and 77 cm$^{-1}$, respectively.

The phonon dispersion, presented in Fig. 4(a), has no unstable modes. This confirms the dynamic stability of single-layer $\beta$-Bi$_2$Pd. There are two low-energy optical branches that start just above 30 cm$^{-1}$ at $\Gamma$ and intersect the acoustic branches going towards the zone boundary. These show substantial electron phonon coupling in the zone, and especially one may note an apparent Kohn anomaly along the $\Gamma$-M line [Fig. 4(a)] with substantial electron phonon coupling. This region provides an approximately 29% contribution to the total $\lambda$. Region III makes the main contribution to the EPC, accounting for approximately 43% of the total $\lambda$. The higher frequency phonons (IV) have a smaller, but non-negligible contribution of 22%. Unlike several other 2D materials, such as borophene, Cu$_2$Si, and Mo$_2$C, the EPC induced by high-frequency phonons is important. As shown in Fig. 4(b), the phonons of regions II and III are mainly from the vibrations of Bi atoms and dominate the EPC of single-layer $\beta$-Bi$_2$Pd.

This provides the ingredients for calculating the transition temperature $T_c$. With a previously used value $\mu^* = 0.1$, we obtain a superconducting transition temperature $T_c = 1.95$ K at ambient pressure, which is smaller than that (4.40 K) of bulk $\beta$-Bi$_2$Pd as obtained by similar methods (see Table...
D. Fermi surface and electronic susceptibility

![Image of Fermi surfaces](image)

**FIG. 5.** Fermi surfaces (a) without and (b) with SOC formed by two bands across the Fermi level in monolayer $\beta$-Bi$_2$Pd.

![Image of electronic susceptibilities](image)

**FIG. 6.** (a) Real part (static or bare) $\chi'(q)$ and (b) imaginary part (Fermi nesting function) $\chi''(q)$ of the electronic susceptibility for single-layer $\beta$-Bi$_2$Pd. (c) and (d) are the corresponding results calculated with SOC. Different colors represent the strength of $\chi'(q)$ and $\chi''(q)$.

The Fermi surfaces of monolayer $\beta$-Bi$_2$Pd are shown in Fig. 5. Without SOC, two bands cross the Fermi level, forming three anisotropic pockets: (i) one concave-square electron pocket at (0,0), (ii) four water-drop shaped hole pockets along the $\Gamma$-M line, and (iii) convex-square hole pockets around the corners. With SOC, the four water-drop electron pockets become four round hole pockets, while the convex-square hole pockets split into an inner and outer section around the M point.

Interestingly, the Fermi surfaces of the hole pockets around neighboring M points are almost parallel to each other. This often gives rise to a Fermi surface nesting and phonon softening, which can contribute to the EPC. The static electronic susceptibility $\chi'$ and the nesting factor $\chi''$ were calculated by extracting the real part and imaginary part of the electronic susceptibility $\chi$ in the constant matrix element approximation. The $\chi'$ is given by

$$\chi'(q) = \sum_k \frac{f(\varepsilon_k) - f(\varepsilon_{k+q})}{\varepsilon_k - \varepsilon_{k+q}},$$

where $\varepsilon_k$ and $\varepsilon_{k+q}$ are band energies measured from the Fermi level at the wave vectors $k$ and $k + q$, respectively. The $\chi''$ is defined by

$$\lim_{\omega \to 0} \chi''(q, \omega) / \omega = \sum_k \delta(\varepsilon_k - \varepsilon_F) \delta(\varepsilon_{k+q} - \varepsilon_F),$$

where $\varepsilon_F$ is the Fermi energy.

Figure 6 shows the resulting $\chi'$ and $\chi''$, calculated on a dense $200 \times 200 \times 1$ k-mesh using the Hamiltonian in the Wannier basis. The inclusion of the SOC leads to a complete reconstruction of the susceptibility around the Fermi level, showing the importance of SOC in this heavy element p-electron system. In the case of $\chi'$ with SOC in Fig. 6(c), the strongest peaks occur along the $\Gamma$-M direction of the Brillouin zone. The softening of the phonons in energy regions I and II mentioned above in the spectrum of Fig. 4(a) may thus stem from this structure in $\chi'$ structure. In addition, $\chi''$ in Fig. 6(d) shows strong peaks around $\Gamma$, which simply reflects the density of states. Other peak positions of $\chi''$ include along the $\Gamma$-X direction. This related to large contributions of $\lambda_{g,n}$ in energy region II seen in Fig. 4(a).

IV. CONCLUSIONS

In summary, starting from the recently discovered topological superconductor $\beta$-Bi$_2$Pd, we investigated the electronic structure and electron-phonon coupling of monolayer $\beta$-Bi$_2$Pd by first-principles calculations. We demonstrate that monolayer $\beta$-Bi$_2$Pd is an intrinsic phonon-mediated superconductor having nontrivial $Z_2$ topology. Therefore, $\beta$-Bi$_2$Pd may be a useful platform for realizing 2D topological superconductivity, and the associated edge states and Majorana physics.

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