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Coexistence of Triple Nodal Points, Nodal Links, and Unusual Flat Bands in intermetallic $\text{APd}_3$ ($A=\text{Pb, Sn}$)

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We investigate the electronic structure and several properties, and topological character, of the cubic time-reversal invariant intermetallic compounds $\text{PbPd}_3$ and $\text{SnPd}_3$ using density functional theory based methods. These compounds have a dispersionless band along the $\Gamma-X$ line, forming the top of the Pd $4d$ bands and lying within a few meV of the Fermi level $E_F$. Effects of the flat band on transport and optical properties have been inspected by varying the doping concentration treated with the virtual crystal approximation for substitution on the Pb site. In the absence of spin-orbit coupling (SOC), we find triple nodal points and three-dimensional nodal loops, which are known to lead to surface bands and drumhead states, respectively, which we discuss for $\text{PbPd}_3$. SOC removes degeneracy in most of the zone, providing a topological index $Z_2=1$ on the $k_z=0$ plane that indicates a topological character on that plane. The isovalent and isostructural compound $\text{SnPd}_3$ shows only minor differences in its electronic structures, so it is expected to display similar electronic, transport, and topological properties.

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I. INTRODUCTION

For the last decade one of the most active issues in condensed matter physics is topological character of the electronic structure and the new properties that may arise. Various types of topological matters have been proposed and some have received experimental support. In addition to topological insulators, three-dimensional topological semimetals have attracted large interest due to their unusual boundary states, which may stimulate novel directions in electronics and spintronics separate from topological insulators. Recently, a novel triple point fermionic phase, having no high energy counterparts, has been also proposed in both nonsymmorphic and symmorphic structures. This phase, predicted along the symmetry line with 3-fold rotation and mirror ($C_{3v}$) symmetries in a few systems of WC-type or half-Heusler structures, is expected to have various unconventional properties and is experimentally observed in MoP.

The intermetallic palladium-lead phase diagram includes various compounds. Among them, the so-called ideal zyryaniteveite compound $\text{PbPd}_3$ (cubic $\text{Cu}_3\text{Au}$ structure) has been investigated as a catalyst for electrochemical oxygen reduction. It has been known that its sister compounds can absorb a large amount of hydrogen, making them of interest as candidates for hydrogen storage or membrane separation.

Separately, flat bands in part or all of the Brillouin zone (BZ) have piqued interest for a variety of reasons. A weakly dispersive band leads to a peak in density of states (DOS), typically much stronger and perhaps narrower than structures arising from van Hove singularities. When a DOS peak is close to, or at, the Fermi level $E_F$, instabilities of the simple Fermi liquid states are encouraged; peaks can enhance a superconducting critical temperature or induce Stoner-type magnetic instability. In $\text{PbPd}_3$ a remarkably flat band appears along the $\Gamma-X$ lines, arising from a lack of $d_{dd}$ hopping such as occurs in (cubic) perovskite-like systems. Because of the limited phase space where the band is flat, it leads to two-dimensional-like step in the DOS (see below). It becomes of importance because it lies within a few meV of $E_F$, implying that transport, thermodynamic, and infrared properties will display unusual dependences on temperature, doping, or other changes in the system (viz. strain).

The manuscript is organized as follows. Sec. II describes our calculational methods based on an $ab$ initio approach. The electronic structure and topological characters of $\text{PbPd}_3$ are presented in Sec. III. Section IV discusses the effects of the unusual flat band on transport and optical properties. A brief comparison of electronic structures between $\text{PbPd}_3$ and $\text{SnPd}_3$ is addressed in Sec. V. Finally, Sec. VI provides a summary.

II. APPROACH

We have performed density functional theory calculations based on the exchange-correlation functional of the Perdew-Burke-Ernzerhof generalized gradient approximation (GGA) with the all-electron full-potential code WIEN2k. Since Pb is a heavy atom, spin-orbit coupling (SOC) is included in all calculations unless otherwise noted. Figure 1 (a) shows the cubic $\text{Cu}_3\text{Au}$ crystal structure (space group: $Pn\bar{3}m$, No. 221), with experimental lattice parameters of $a = 4.035$ Å for $\text{PbPd}_3$ and $a = 3.971$ Å for $\text{SnPd}_3$. Both experimental parameters are smaller by about 2% than our values optimized in GGA. Here, our calculations were based on the experimental values, unless mentioned otherwise.

The topological properties were explored by the Wannier function approach. From the band structures ob-
tained from wien2k, Wannier functions and the corresponding hopping amplitudes were generated using the wannier90\textsuperscript{25} and wien2wannier\textsuperscript{26} programs. The surface spectral functions were calculated by the wannier90\textsuperscript{25} code.\textsuperscript{27} The transport and optical properties were calculated by two extensions of wien2k. Based on the semiclassical Boltzmann transport theory with a constant scattering time approximation, the transport calculations were carried out with the boltztrap code.\textsuperscript{28} Calculation of optical properties including SOC is available in the optics.\textsuperscript{29} Assuming an inverse scattering lifetime $\gamma = 10$ meV in the intra-band contribution, the dielectric function $\epsilon(\omega)$, contributed by both intra- and inter-band excitations, was calculated. The electronic energy loss function is given by $-\text{Im}[\epsilon^{-1}(\omega)]$.

In wien2k, the BZ was sampled by a very dense $k$-mesh $40 \times 40 \times 40$ due to its sharp DOS structure near $E_F$. For a careful check of the position of the flat band, a high value of basis set cutoff $R_{\text{mt}} K_{\text{max}} = 9$ was used to determine the basis size with atomic radii of 2.5 bohr for the both ions.

III. ELECTRONIC AND TOPOLOGICAL CHARACTERS OF PbPd\textsubscript{3}

A. Electronic structure of PbPd\textsubscript{3}

The band structures of both GGA and GGA+SOC near $E_F$ are shown in Figs. 2(a) and 2(b). In this energy regime, the bands have mostly Pb 6s, 6p above $E_F$ and Pd 5d character below. The corresponding density of states (DOS) with Pd 5d orbital-projected DOS is given in Fig. 2(c).

The band structure shows unusual characteristics relating to transport, thermodynamic, and topological properties. Most prominently, a very flat band of Pd 5d character appears along the $\Gamma - X$ line only a few meV above $E_F$. The lack of dispersion reflects the lack of nearest neighbor (NN) Pd $dd\delta$ hopping. This characteristic appears commonly in cubic perovskite-related systems,\textsuperscript{19} but is unusual in intermetallic compounds. As indicated in Fig. 2(a), for the $\Gamma - X$ line along the (100) direction, the flat band has solely the $d_{yz}$ orbital character of Pd\textsubscript{2} $[(\frac{1}{2}, \frac{1}{2}, 0)]$ and Pd\textsubscript{3} $[(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})]$ ions. Significantly, in PbPd\textsubscript{3} this flat band lies only 6 meV above $E_F$, thereby giving an effective Fermi energy for holes of $E_{F, h} = 6$ meV and corresponding Fermi temperature $T_{F, h} = 70$ K. As can be seen in Fig. 2(c), structure in the DOS is a 2D-like step discontinuity, and electron doping of only $\sim 0.01$ carrier/f.u. would be required to move $E_F$ up to the band edge. Above the edge, the DOS is very small (semimetal-like) up to 0.2 eV.

Another aspect that we will follow is an occurrence of 3-fold degeneracies along symmetry lines, which are becoming known as triple nodal points (TNPs). In the absence of SOC, as shown in Fig. 2(a), spinless TNPs $\Gamma_{\text{13}}$ appear at the $\Gamma$ point. Along the $\Gamma - R$ line, having the $C_{3v}$ symmetry, the $\Gamma_{\text{14}}$ band at 0.1 eV splits into a doublet $\Lambda_1$ of a positive effective mass and a singlet $\Lambda_2$ of a negative effective mass. The $\Gamma_{\text{14}}$ band slightly above $E_F$ splits into a doublet $\Lambda_1$ and a singlet $\Lambda_2$, both with negative effective masses. As previously noted,\textsuperscript{2,3} the $\Lambda_3$ and $\Lambda_4$ crossing forms a TNP at $(0.39, 0.39, 0.39)_{\text{\AA}}^2$ at 0.15 eV along the $\Gamma - R$.

At the $R$-point, a TNP of $R_{\text{14}}$ symmetry lies at $-0.32$ eV. This band splits into a doublet $T_5$ of a positive effective mass and a singlet $T_2$ along the $R - M$ line, having $C_{4v}$ symmetry. This doublet forms a TNP with the $T_4$ at $(\frac{1}{2}, \frac{1}{2}, 0.312)_{\text{\AA}}^2$ at 0.19 eV. The TNP along the $C_{4v}$ symmetry line has not been discussed previously. One may expect surface states connecting these spinless TNPs in the absence of SOC. The surface states for PbPd\textsubscript{3} are discussed below.

In addition to TNPs, there is a nodal point at $\sim 0.5$ eV along the $R - M$ line at $(\frac{1}{2}, \frac{1}{2}, 0.3983)_{\text{\AA}}^2$. Perpendicular to this line and along cubic directions, this double degeneracy does not split, forming the three interconnected topological nodal loops shown in Fig. 3(c). The three nodal loops lie on mutually perpendicular mirror planes. These $R$-centered links are similar to what was reported in the antiperovskite Cs\textsubscript{3}PdN.\textsuperscript{30}

To probe the origin and sensitivity to symmetry lowering of these TNPs, the cubic structure has been distorted, conserving the volume. Tetragonal distortion leads to breaking $C_{3v}$ symmetry, thereby removing TNPs along the (111) direction. Both the $C_{3v}$ and $C_{4v}$ symmetries are broken by orthorhombic distortion, resulting in the vanishing of the TNPs along both the $R - M$ line as well as along the (100) directions. See the Supplemental Material for additional information.\textsuperscript{31} These TNPs are protected by the mirror plus three-fold, or four-fold, rotational symmetries respectively.

Comparison of the two band structures without and with SOC in Fig. 2 reveals several effects of SOC. SOC
leads to anticrossing of several, but not all, crossing bands, as well as lowering the flat band toward $E_F$, from 15 meV to 5 meV. At the $\Gamma$ point, two 6-fold degenerate bands $\Gamma_{4\pm}$ (including spin) split into doublet and quartet, resulting in a SOC gap of 0.3 eV due to a band inversion. Substantial impacts of SOC resulting in changes of surface states appear in the spinless TNPs along $\Gamma - R - M$ lines near the $R$-point at $\sim 0.2$ eV. As discussed by Zhu and coworkers, these TNPs are not protected in the cubic structure, when including SOC. Instead, SOC driven anticrossings at these TNPs lead to eight symmetry related fourfold degenerate Dirac points at $\sim 0.2$ eV along $\Gamma - R$, and six at $\sim 0.15$ eV along $R - M$. A similar behavior along a $C_6v$ line was suggested in the layered hexagonal AlB$_2$-type metal diborides. Thus the band structure is gapped at 0.2 eV except for the band emanating from $R$, strengthening the semimetal viewpoint of the near-$E_F$ electronic structure of PbPd$_3$.

One result of this semimetallic band structure is delicate Fermi surfaces (FSs). Figure 3 displays the physical FSs (SOC included), consisting of three types. Narrow cylindrical open hole FSs lie along the $(100)$ axes, intersecting at the zone center; these tubes are related to the flat band along $\Gamma - X$ discussed above. An $R$-centered electron spheroid FS has a radius of $0.26(2)$, containing 0.03 electrons per formula unit. Additionally, there are tiny elliptical hole pockets ("carrots") around this sphere along the $(111)$ directions and tiny spheroids along the $(100)$ directions.

Most results obtained for our optimized lattice parameter are very close to those for the experiment parameter presented above, as expected from the fact that the difference is small (less than 2%). There is however a distinction worth mentioning. For the optimized (larger) volume, the flat band is shifted to $-5$ meV relative to $E_F$. Thus modest pressure can be used to tune this
B. Topological character of PbPd$_3$

Using a Wannier representation of the bands, we have carried out surface calculations based on the Green function approach$^{32}$ for a semi-infinite crystal. For PbPd$_3$, there are two possible (001) surface terminations, one containing both Pb and Pd atoms (Pb-Pd) and the other containing only Pd surface atoms (Pd$_2$). Figure 4 shows the surface spectral functions for the each termination, in both GGA and GGA+SOC. Around 0.2 eV above $E_F$, the surface zone is gapped except around the $\bar{M}$ point, arising from the bulk bands around $R$ that project onto $\bar{M}$. In the absence of SOC, in Figs. 4(a) and (c) the Pd$_2$ termination shows a weakly dispersive surface band in both directions from $\bar{\Gamma}$. For the Pb-Pd terminated surface only surface resonances within the bulk bands appear along symmetry lines. Several surface states appear at the projections of TNPs both in the gap and inside the bulk states in both terminations. The positions of TNPs and their projections onto the surface BZ are provided in Fig. 1(b). At $\bar{\Gamma}$ there is a surface band $\sim$ 15 meV above $E_F$, corresponding to the TNP at $\bar{\Gamma}$ at 16 meV that projects onto $\bar{\Gamma}$. One of the TNPs (at 0.2 eV) along the $R - \bar{M}$ line projects onto $\bar{M}$, and any surface states that might be related are hardly evident, as it is within a strong background of projected bulk states around $\bar{M}$. The other two TNPs project onto the $\bar{M} - \bar{X}$ line, where a strong surface band appears within the gap at 0.1-0.3 eV, but only for the Pd$_2$ termination. This strong surface band is seen everywhere within the gap. Since it is missing for the PbPd terminated surface, its relation to TNPs is in doubt.

SOC is known to have strong consequences in nodal point and nodal loop materials. Inclusion of SOC leads to a large 0.4 eV gap just above $E_F$ at the $\Gamma$ point and all along the $\Gamma - X$ line, hence a 0.4 eV gap at $\bar{\Gamma}$, resulting in qualitative changes in the surface spectrum. As shown in Fig. 4(b), in the Pd$_2$ termination the surface band in the absence of SOC becomes two surface bands, separated by a 0.4 eV gap around $\bar{\Gamma}$ point but connecting valence and conduction bands. These bands merge at $\bar{X}$ and also as they enter the bulk spectrum along the other two symmetry lines.

For Pb-Pd termination, where no surface bands around $\bar{\Gamma}$ appear within the gap in GGA, SOC produces a new occurrence, one that is very different from that of the...
FIG. 5: Spectral densities of the surface Fermi contours of the surface states shown in Fig. 4, for (top) Pd$_2$ and (bottom) Pb-Pd terminations. The left panels are for GGA only, the right panels show results for GGA+SOC. The strong yellowish lines denote surface bands.

FIG. 6: Plot of the hybrid Wannier charge centers (WCCs) plot (red, thick lines) across half of the Brillouin zone in the $k_z = 0$ plane, showing an odd number of crossings between the charge center and largest gap among two adjacent WCCs. The gap function is designated by the blue (thin) line. The magnitude of the wave vector $k_y$ in the horizontal axis is given in units of $\pi/a$.

Pd-Pd termination: a surface band Dirac point emerges at $\bar{\Gamma}$ at 0.25 eV above $E_F$ from two linear bands joining valence to conduction bands, as shown in Fig. 4(d). This surface crossing is enabled by SOC opening a bulk gap at $\Gamma$. In the Pb-Pd termination, a 2D Dirac cone at the $\bar{\Gamma}$ point is a dominant feature. In Fig. 4 (e,f) the spin textures are shown for cross sections of the cones just above, and just below, the Dirac point. The orientation of texture is in opposite helical direction in the upper and lower cones, reflecting the topological character of this point.

C. Fermi level spectral density

The surface Fermi level spectral density contours (the surface Fermi lines) are pictured in Fig. 5, presented analogously to Fig. 4. As expected from differences between the two terminations in the surface spectrum, a clear distinction appears along the $\bar{\Gamma} - \bar{X}$ line, whereas features around $\bar{M}$ are nearly identical. For Pd$_2$ termination there are four symmetry related ovoid pockets along the axes, both without and with SOC. These are shown in Fig. 5 (a) and (b), indicating that SOC substantially increases the area of these pockets (increases the density of the corresponding carriers). The bulk $R$ point and its Fermi spheroid project onto the $\bar{M}$ point, and protrusions along axes and diagonals connected to this spheroid appear for both terminations. There is only small quantitative change with SOC. For higher resolution figures, see the Supplemental Material.

Calculations of the hybrid Wannier charge centers (WCCs) allow a “theoretical spectroscopy” of topological character in cases where the full zone is not gapped. In this technique, the Bloch-to-Wannier transformation is applied only to one direction, and in cubic crystals there is only one choice of direction. These calculations were performed to establish topological character using the wanniertools code. In this method, the $Z_2$ number is calculated from the number of crossings of WCCs mod 2 by an arbitrary line in half of BZ, making use of time-reversal symmetry. As a practical matter, instead of an arbitrary line, a line between two adjacent WCCs is chosen for numerical efficiency.

In PbPd$_3$, inclusion of SOC separates bands over most of the BZ, band crossings surviving only around the $R$ point. Thus the electronic structure on the basal planes (viz. $k_z = 0$) can be considered as insulating subspaces, thus providing a well-defined $Z_2$ number that can be calculated using the WCC method. As shown in Fig. 6, there is an odd number of crossings of the largest gap with the charge centers, giving $Z_2=1$. This number is also obtained from parities of all occupied eigenstates at time-reversal invariant momenta in the $k_z = 0$ plane. The parities are given by $-1$ at $\bar{\Gamma}$ and $+1$ at $X$ and $\bar{M}$, for a product of $-1$, again indicating $Z_2=1$. Therefore this crystal is a topological insulator on the $k_z = 0$ plane.

D. Strain effects

We have considered tetragonal and orthorhombic distortions to investigate effects of strain. The $Z_2$ indices are well defined in both $k_z=0$ and $\pi/c$ planes in both cases even for a small strain. Due primarily to a change of parity at $\bar{\Gamma}$, the corresponding indices are 0;[0,0,0] for the both cases, indicating a topologically trivial phase. How-
ever, in-gap surface states appear, similar to the topological crystalline insulating phase proposed in the tetragonal lattice\textsuperscript{37} or the orthorhombic perovskite iridates.\textsuperscript{38}

For more information see the Supplemental Material.\textsuperscript{31}

Two sister compounds, semimetallic SnPd\textsubscript{3} and PbPd\textsubscript{3}, are worthy of comment. In contrast to the Pd analogies with several TNPs above \(E_F\), the valence bands are fully filled, so SOC leads to well separated bands around \(E_F\) throughout the BZ.\textsuperscript{39} SnPd\textsubscript{3} has been proposed as a weak topological insulator,\textsuperscript{40} while PbPd\textsubscript{3}, with its additional complexities, will be discussed elsewhere.\textsuperscript{39}

IV. ROLE OF THE FLAT BAND; ELECTRON DOPING

We have varied the electron concentration in \((\mathrm{Pb}_{1-x}\mathrm{Bi}_x)\mathrm{Pd}_3\), which is experimentally accessible,\textsuperscript{22} to inspect the role of the flat band in transport and optical properties, using the virtual crystal approximation, for which this is an optimal application. We will focus on GGA+SOC results. There is negligible change in band structure, and Fig. 7 displays the rising of the Fermi level with added electrons. The flat band precisely lies at \(E_F\) for \(x = 0.01\), and by \(x = 0.02\) the intersecting cylinder FSs disappear. At \(x = 0.03\), the hole pockets at the \(\Gamma\) point are filled. Since transport and optical properties are derived from the bands \(\varepsilon_k\), its derivatives, and the Fermi level position,\textsuperscript{41} one may anticipate specific features related with the flat band in PbPd\textsubscript{3}. These properties are surveyed in the following subsections.

A. Transport properties

The transport properties have been calculated based on quasiclassical Bloch-Boltzmann transport theory,\textsuperscript{41} assuming a constant scattering time \(\tau\) approximation.

Our results including SOC are pictured in Fig. 8. The Hall coefficient \(R_H(T)\), given in Fig. 8(a), shows substantial variation with temperature even at these very low doping levels. At zero doping \(x=0\), it is net (from competing Fermi surfaces) electron-like in sign. With increasing \(T\), \(R_H(T)\) monotonically decreases, and just above 800 K crosses zero, where electron and hole contributions compensate. With increasing doping, \(R_H(T)\) crosses zero at lower temperatures, \(e.g.,\) for \(x = 0.03\) exact compensation of holes and electrons occurs at 400 K. For \(x = 0.033\), \(R_H(T)\) is negative for the whole range of \(T\), indicating dominance of hole carriers. Recall however that in a multiband system \(R_H(T)\) has no simple relation to carrier densities.\textsuperscript{42}

Figure 8(b) shows the \(T\)-dependent conductivity over scattering time \(\sigma/\tau\). For a typical metal with large \(N(E_F)\), \(\sigma/\tau\) is proportional to \(N(\mu)\langle v_F^2\rangle\)\textsuperscript{43} with insignificant \(T\)-dependence. Here \(N(\mu)\) and \(\langle v_F^2\rangle\) are the DOS at the chemical potential \(\mu(T)\) and the thermal average of square of the Fermi velocity at \(\mu(T)\), respectively. With structure in \(N(E)\) around \(E_F\), \(\mu\) becomes \(T\)-dependent. As \(T\) rises above 400 K \((x=0)\), \(\sigma/\tau\) increases, by about 25% at 800K, due to the sharp drop in \(N(E)\) at 6 meV above \(E_F\). As doping increases, the low temperature value drops and the temperature increase is enhanced as \(E_F\) moves upward with doping, through the DOS singularity and into the semimetal region.

Related variations are reflected in the Seebeck coeffi-
FIG. 9: Energy loss function $L(\omega)$ versus energy $\omega$ ($\hbar=1$), for the various electron-doping levels. A scattering rate $\gamma = \hbar/\tau$ of 10 meV has been assumed, which primarily affects the widths of peaks but also determines the (small) intraband contribution. Inset: Enlarged plot below $\omega = 0.4$, showing the low energy plasmonic peak(s) clearly. For $x=0$, the result without SOC is included to indicate the influence of SOC in the loss function.

The electron energy loss function $L(\omega)$, given in Fig. 9, was calculated as the imaginary part of the inverse dielectric function $\varepsilon(\omega)$. The dielectric function includes both intra- and interband contributions. In the intraband part, containing the Drude term, an inverse scattering time $\tau$ is chosen from $\gamma = \hbar/\tau = 10$ meV.

**B. Optical properties**

The overall behavior of $L(\omega)$ is non-monotonically dependent on electron-doping level. PbPd$_3$ is a nearly transparent (semi)metal in the far infrared region $\omega < 75$ meV. At zero doping, the large loss peak at 0.2 eV when SOC is neglected is split by SOC, leaving a series of less pronounced subpeaks at 0.11, 0.14, and 0.27 eV. The plasmon peak around 0.1 eV is mainly due to excitation at the $\Gamma$-point and has the strongest intensity at $x = 0.03$. The intensity and position of these peaks depends somewhat on the choice of $\gamma$.

**V. THE Sn ANALOG**

Isovalent and isostructural SnPd$_3$, with a 1.5% smaller lattice constant than PbPd$_3$, was also investigated. As expected, the band structure of SnPd$_3$, presented in Fig. 10(a), is very similar to that of PbPd$_3$, using GGA only. However, in SnPd$_3$ effects of SOC are not as substantial as in PbPd$_3$, since the strength of SOC in Sn is weaker than in Pb. The GGA+SOC band structure and the corresponding DOS are displayed in Figs. 10(b) and (c). Compared to PbPd$_3$, there are two distinctions worth noting. First, the flat band, which is shifted downward by SOC, lies at 10 meV versus 6 meV for PbPd$_3$. Second, the bottom conduction band lies very close to, but above, $E_F$ along the $\Gamma - R$. These two features result in change in fermiology of SnPd$_3$, shown in Fig. 3(b) beside that of PbPd$_3$. The radius of the pipe-like FS is increased and irregular rod-shape FSs appears along the $\{111\}$ directions.

**VI. SUMMARY**

Using various calculations based on \textit{ab initio} approach and semiclassical Bloch-Boltzmann theory, we have investigated the peculiar electronic structure, topological characters, and some transport characteristics of intermetallic PbPd$_3$, which has a very flat band along the $\Gamma - X$ line nearly coinciding with the Fermi level. In the absence of SOC, several triple points emerge near $E_F$ along the $C_{3v}$ and $C_{4v}$ symmetry lines, leading to surface...
Dirac cones along the $\Gamma - \bar{M}$ lines and Fermi arcs around the zone corner on the surface states. Nodal points along the $M - R - M'$ line lead to three dimensional nodal links that lie on mirror planes. SOC removes degeneracies in most of the zone, leading to a topological insulating phase on the $k_z = 0$ plane. We have furthermore inspected effects of the unusual dispersionless band on transport and optical properties by varying the doping level.

Although there are some distinctions due to difference in strength of SOC between Pb and Sn ions, most of the electronic structure characteristics of PbPd$_3$, including the flat band, are shared with isovalent and isostructural SnPd$_3$, suggesting it will display similar transport, optical, and topological properties.

VII. ACKNOWLEDGMENTS

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31. See Supplemental Material at URL for the band structures and HWCCs of the distorted structures, the blowup surface spectral functions.


