Hidden type-II Weyl points in the Weyl semimetal NbP

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As one of Weyl semimetals discovered recently, NbP exhibits two groups of Weyl points with one group lying inside the $k_z = 0$ plane and the other group staying away from this plane. All Weyl points have been assumed to be type-I, for which the Fermi surface shrinks into a point as the Fermi energy crosses the Weyl point. In this work, we have revealed that the second group of Weyl points are actually type-II, which are found to be touching points between the electron and hole pockets in the Fermi surface. Corresponding Weyl cones are strongly tilted along a line approximately $17^\circ$ off the $k_z$ axis in the $k_x - k_z$ (or $k_y - k_z$) plane, violating the Lorentz symmetry but still giving rise to Fermi arcs on the surface. Therefore, NbP exhibits both type-I ($k_z = 0$ plane) and type-II ($k_z \neq 0$ plane) Weyl points.

I. INTRODUCTION

Weyl semimetals (WSMs) were recently found in four transition-metal monopnictides, TaAs, TaP, NbAs and NbP, by theoretical predictions and angle-resolved photoemission spectroscopy (ARPES). In the bulk, these materials exhibit Weyl points through which conduction and valence bands cross each other linearly in the three-dimensional momentum space. At the Weyl point, the Fermi surface usually shrinks into a point. The quasi-particle excitations near the Weyl point behave effectively as a kind of massless relativistic particles known as Weyl fermions in the standard model. These Weyl points are monopoles of the Berry curvature field and thus lead to topological boundary states on the surface. The topological surface state connects a pair of Weyl points with opposite chiralities, resulting in an unclosed curve in the Fermi surface, called the Fermi arc. The type-II WSM exhibit a very different Fermi surface from a normal WSM (referred to as type-I) at the Weyl point. It has finite Fermi pockets, where the touching point between the electron and hole pockets is the type-II Weyl point. Although it also exhibits Fermi arcs, the type-II Weyl cone is expected to demonstrate direction-dependent chiral anomaly effect and optical response, and even catalysis.

Very recently a new type of WSMs were anticipated and discovered in MoTe$_2$, called the type-II WSM. The Weyl cone is strongly tilted so that the Fermi velocity reverses its sign along the tilting direction (see Fig. 1). The type-II WSM exhibit a very different Fermi surface from a normal WSM (referred to as type-I) at the Weyl point. It has finite Fermi pockets, where the touching point between the electron and hole pockets is the type-II Weyl point. Although it also exhibits Fermi arcs, the type-II Weyl cone is expected to demonstrate direction-dependent chiral anomaly effect and large photocurrent.

II. METHODS

The band structure calculations were performed with the density-functional theory within the generalized gradient approximation, which is implemented in the Vienna ab-initio simulation package (VASP). The SOC was included. We project the ab initio wave functions that a group of Weyl points in NbP, which has the weakest SOC among four compounds, are actually type-II by bulk and surface band structure calculations. This fact is overlooked in previous research, mainly because these Weyl points lie above the Fermi energy and cannot be directly accessed in ARPES and transport measurements, and also because the tilting direction of the Weyl cone is away from ordinary crystallographic axes.
to the localized Wannier function\textsuperscript{13} and constructed the tight binding Hamiltonian for bulk NbP, to interpolate the band structure and Fermi surface in the Brillouin zone by dense \( k \)-grids. For the surface states, we used two models. One is a semi-infinite surface model constructed by the tight-binding parameters based on the bulk Wan-ner orbitals. The other is a slab model with a thickness of 15 bulk unit-cells, calculated in a fully \textit{ab initio} way. Two models give different Fermi arc states due to different boundary conditions, but exhibit the same topology in the Fermi surface.

III. RESULTS

The energy dispersion of NbP presents as a semimetallic state with tiny electron and hole pockets cutting the Fermi level. Due to inversion symmetry breaking, spin degeneracy splits for all the bands\textsuperscript{7,8}, as shown in Fig. 2(a). Based on the calculated band structure we have achieved good agreement with experimental magnetic quantum-oscillation measurements, which confirmed the accuracy of our calculations\textsuperscript{7,7,8,11}. Consistent with previous reports, there are totally twelve pairs of Weyl points in the whole Brillouin zone (BZ), with four pairs in the \( k_z = 0 \) plane (W1) and the others in the plane around \( k_z \sim \pm \pi/c \) (W2), which are 57 meV below and 5 meV above the Fermi level in energy space, respectively\textsuperscript{7,7,8,11}. The Fermi surface topology revealed that W1-type Weyl points are type-I\textsuperscript{7,7,8,11}.

The energy dispersion crossing the W2 Weyl point along high symmetry directions of \( k_x, k_y \) and \( k_z \) present very good type-I features, as presented in Fig. 2(b-d). That should be a simple reason why W2 Weyl points was assumed to be a type-I. However, it cannot exclude the possibility that the W2 Weyl cone is strongly tilted along some low-symmetric direction.

For further identifying the feature of the Weyl point in NbP, we analyzed the Fermi surface accordingly. As it is already known from quantum oscillation and previous calculations, when the Fermi level is 5 meV below Weyl points, both of the electron and hole pockets present as banana shape with strong anisotropy\textsuperscript{7,7,8,11}. The Fermi surfaces can be separated into two branches in the reciprocal space without any touching point. However, if we shift up the chemical potential exactly to the energy of W2 Weyl points, it is found that electron and hole pockets touches each other in \( k_z \sim \pm \pi/c \) planes. Here, W2 Weyl points are exactly the touching points, presenting clearly a type-II feature. Taking the Fermi surfaces with \( M_y \) symmetry as the example, Fig. 3(a), we can see that the electron and hole pockets linear touching each other along the direction of 17° off the \( k_z \) axis. So the Weyl cone is strongly tilted in the \( k_y = k^W_y \) planes (the position of Weyl point W2 is \( k^W_x, k^W_y, k^W_z \)). As shown in Fig. 3(b), The 2D cross-section of Fermi surfaces in \( k_y = k^W_y \) plane forms a linear crossing but not shrink to a point. We also analysed the energy dispersion crossing the Weyl point along the titled direction, Fig. 3(c), which is completely different from that along high symmetry lines as given in Fig. 2(b-d).

The type-II Weyl point is further confirmed by the surface state. Though both type-I and type-II Weyl points can induce the non-closed surface Fermi arc, the shapes of them are different. In type-I WSMs, the bulk Fermi surface shrinks to a point at Weyl point. Hence, when the energy is fixed at the Weyl point, the Fermi arc will terminate at two isolated points without any bulk density of states. While in type-II WSMs, one can expect to observe the linear touching of surface projected electron and hole pockets at the Weyl points, where are terminations of the Fermi arcs. In general, anion-terminated (P) surface in (001) direction was usually reported for the as-cleaved surface in ARPES for NbP\textsuperscript{12,13}. Since NbP is not a layered material, the chemical bonding is very strong, and the charge redistribution plays an important role for the detailed shape of the surface Fermi arc states. Therefore, in this work we have first analysed the surface state by a tight-binding semi-infinite model, which provides a clear understanding of the topological Fermi arc state. Further, we also studied the surface state with surface charge redistribution taken into account by fully \textit{ab-initio} slab calculations. Tight-binding and \textit{ab-initio} show different surface states, but the same topology.

For convenience we just focus on one pair of Fermi arcs near the \( M_y \) mirror plane. The surface band structure with P termination along \( k_y \) with fixed \( k_y = k^W_y \) is given in Figure 3(a). Since two pairs of W2 points with the same chirality are projected to the same point in the (001) 2D BZ, two Fermi arcs are expected from one pair of projected Weyl points. From surface energy disper-
FIG. 3. (a) Eight pairs of Weyl points are denoted by green and yellow dots to represent opposite chirality of type-II Weyl points, and four pairs of Weyl points are denoted by blue and red dots to represent opposite chirality of type-I Weyl points. Red and green pockets represent hole and electron pockets, respectively. The black dash line indicates the special direction for non-chiral anomaly. (b) The 3D band structure of the W2 Weyl cone in the $k_x$-$k_z$ plane is heavily tilted, which shows the type-II character of the W2 nodes in NbP. The energy contour at the bottom corresponds to the Fermi level at W2 Weyl point. Two bands of upper and lower cones are indicated as green and red lines. The tilted line in (a) is also projected into the contour. (c) The band structure along the tilted line in (a). The cross-section of the 3D band structure shows that the W2 node lies 5 meV above the intrinsic Fermi level $E_f$ (neutral). $k$ coordinates are in unit of reciprocal vectors.

FIG. 4. (a) The band structure along $\bar{k}_x$ ($\bar{k}_y = 0.0048$) and (b) the Fermi surface of the semi-infinite surface. (c) The Fermi surface of slab model by DFT. The gray region is bulk states. $k_x$ and $k_y$ are in unit $2\pi/a$.

IV. SUMMARY

In conclusion, we have predicted the existence of type-II Weyl fermions in NbP based on electronic band structure calculations. We revealed that the Weyl cone is tilted strongly along a specific direction, breaking the Lorentz symmetry. Since the tilting direction is away from ordinary $a$ and $c$ axes, one may still expect the chiral anomaly effect along $a$ or $c$ directions. Since the type-II Weyl point is only 5 meV above the Fermi level, weakly electron doping may lead to the observation of the type-II Weyl points by ARPES.
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