Type-II Dirac Nodal Lines in a Double-Kagome-Layered Semimetal

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Lorentz-violating type-II Dirac nodal line semimetals (DNLSs), hosting curves of band degeneracy formed by two dispersion branches with the same sign of slope, represent a novel state of matter. While being studied extensively in theory, convincing experimental evidence of type-II DNLSs remain elusive. Recently, vanadium-based kagome materials have emerged as a fertile ground to study the interplay between lattice symmetry and band topology. This work studies the low-energy band structure of double-kagome-layered CsV$_8$Sb$_{12}$ and identifies it as a scarce type-II DNLS protected by mirror symmetry. This work observes multiple DNLSs consisting of type-II Dirac cones close to or almost at the Fermi level via angle-resolved photoemission spectroscopy (ARPES), which provides an electronic explanation for the nonsaturating magnetoresistance effect as observed. First-principles theory analyses show that spin-orbit coupling only opens a small gap, resulting in effectively gapless ARPES spectra, yet generating large spin Berry curvature. These type-II DNLSs, together with the interaction between a low-energy van Hove singularity and quasi-one-dimensional band as observed in the same material, suggest CsV$_8$Sb$_{12}$ as an ideal platform for exploring novel transport properties.

1. Introduction

In three-dimensional materials, the band crossing between valence band and conduction band can form discrete points, described as Dirac semimetals and Weyl semimetals.[1] The bands can also cross along a curve, described as Dirac and Weyl nodal-line semimetals (DNLSs and WNLSs).[2–4] In general, DNLSs can be categorized into type-I and type-II,[5,6] according to the band dispersion slope around the band crossing. In type-II semimetals, the asymmetric valence and conduction bands induced by the tilted linear dispersion lead to the coexistence of electron and hole pockets on the Fermi surface, and thus exhibit large unsaturated magnetoresistance (MR), as found in WTe$_2$[7] and Mg$_3$Bi$_2$.[8] Compared with type-I DNLSs, type-II DNLSs host other distinct

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Crystal structure, band structure, and magnetotransport of CsV₈Sb₁₂. a) Lattice structure of CsV₈Sb₁₂, conventional cell. Cs, V, and Sb atoms are represented by green, blue, and brown balls, respectively, where the V atoms in the kagome V₃Sb layer and orthorhombic V₂Sb₂ layer are labeled as V₁ and V₂. b) First (solid black lines) and second (dashed blue lines) Brillouin zones (BZs) of CsV₈Sb₁₂ primitive cell. c) Density functional theory (DFT) calculated band structure along high-symmetry paths. d) Temperature dependence of $\rho_{xx}(T)$ at zero field of CsV₈Sb₁₂. e) Field dependence of magnetoresistance (MR) with $I//a$ and $H//a$ at 2 K.

2. Results and Discussion

CsV₈Sb₁₂ adopts an orthorhombic lattice with space group of Fmmm. Both AV₃Sb₅ and CsV₈Sb₁₂ share a common V₃Sb₅ unit that consists of a V-based kagome layer V₁Sb sandwiched by two Sb₂ honeycomb lattices. While AV₃Sb₅ has one V₁Sb₅ unit, CsV₈Sb₁₂ has two V₁Sb₅ units, plus an orthorhombic V₂Sb₂ layer in between (Figure 1a). Considering the mirror symmetry in the $z$ direction, the effective unit cell (red dashed box in Figure 1a) with $c = 18.1$ Å consists of two [half Cs-V₁Sb₅-half V₂Sb₂] units (blue dashed box) that are related to each other by glide plane. This sublattice symmetry leads to an apparent periodicity of $4\pi/c$ as shown in Figure 4a. The apparent doubling of the $k_z$ periodicity as a consequence of the nonsymmetric lattice structure is also observed in other materials, such as graphite[30] and BiTeCl.[40] With the first and second Brillouin zones (BZs) shown in Figure 1b, Figure 1c demonstrates the DFT calculated band structure of CsV₈Sb₁₂. There are many bands

properties, e.g., magnetic field direction-dependent chiral anomaly,[9] magnetic breakdown, and the Klein tunneling.[10] Although quite a lot of theoretical efforts have been made on the prediction of the type-II DNLSs,[5,6,11–14] the direct spectral evidence to realize the type-II DNLS phase in these materials is still missing.

AV₃Sb₅ ($A = K, Rb, Cs$) family of materials[15–17] intertwine charge density wave (CDW), superconductivity and band topology, exhibiting novel properties such as pair density wave,[18] giant anomalous Hall conductivity,[19,20] time-reversal symmetry breaking (TRSB) and possible chiral flux phase.[21–24] Topological band features, such as van Hove singularity (VHS) and Dirac nodal loop,[25–31] are observed and fundamental to shape those properties. However, despite intensive research efforts, there are still controversies concerning the existence of chiral flux phase, the chirality of CDW and its relationship with TRSB and VHSs.[32,33] Recent efforts[34,35] have succeeded in synthesizing double-V-kagome-layered materials CsV₈Sb₁₂, which offers a great chance to design controllable experiment to study the origin of the exotic properties as mentioned above. While CsV₈Sb₁₂ has been thoroughly studied, the band structure topology of double-kagome-layered CsV₈Sb₁₂ remains to be clarified experimentally.

In this work, we identify double-kagome-layered CsV₈Sb₁₂ as a type-II DNLS. Combining photon energy-dependent ARPES measurement and density-functional theory (DFT) analyses, we have observed multiple groups of type-II DNLs extending along $k_z$ direction, which are protected by mirror symmetry and lying close to or almost at the Fermi level. The coexisting electron and hole Fermi pockets of type-II Dirac cones feature a linear non-saturating MR in our magnetotransport measurements. According to DFT, spin-orbit coupling (SOC) only opens a very small gap at the band crossings, effectively yielding gapless DNLs in the ARPES spectra yet large spin Berry curvature. We have also observed low-energy VHS interacting with a quasi-one-dimensional (quasi-1D) band, both featuring enhanced density of state. The identification of type-II DNLs provides a clear picture to categorize the band structure topology of double-kagome-layered CsV₈Sb₁₂, and the intrinsic, low-energy electronics features may stimulate further transport exploration for novel topological and correlated physics[9,10,36–38] in V-based kagome materials.
crossing the Fermi level, forming multiple Dirac cones in a shallow region below $E_F$. The resistivity measurements (Figure 1d) exhibit a metallic-like behavior and no superconductivity or CDW transition is found in CsV$_8$Sb$_{12}$, consistent with the previous results.[34,35] The magnetic-field-dependent MR (defined as $\rho(H)/\rho(0)$, where $\rho$ is the resistivity under an applied magnetic field $H$) for $H//a$ and $I//a$ is shown in Figure 1e. The MR increases with the magnetic field gradually, and above 5 T, increases linearly without any signs of saturation up to 14 T at 2 K, which is different from the saturation behavior of another MR result on the same material.[34] The MR reaches about 120% under 14 T. Similar to the case of WTe$_2$[8] and NbP,[41] the non-saturating MR behavior may originate from the coexistence of electron and hole Fermi pockets induced by the type-IID Dirac cones. ARPES measurements are then conducted to investigate the detailed electronic structure of CsV$_8$Sb$_{12}$.

Figure 2 demonstrates the measured and calculated Fermi surfaces and band dispersions of CsV$_8$Sb$_{12}$. Satisfactory agreements between ARPES measurements and DFT calculations are reached concerning the general symmetry and detailed band structure. Because of the orthorhombic V$_2$Sb$_2$ layer, the symmetry of CsV$_8$Sb$_{12}$ is reduced to $D_{2h}$, in contrast to the $D_{6h}$ symmetry in AV$_3$Sb$_5$. In line to this, the Fermi surface and constant energy contours (CECs) (Figure 2a–d) both show twofold symmetry, with spectral features symmetric to $Z-A$ and $Z-T$ lines. ARPES spectra and DFT dispersions along these two high-symmetry paths are shown in Figure 2e–h for comparison. The ARPES-measured electronic features of CsV$_8$Sb$_{12}$ can be roughly categorized into three groups: multiple (gapped) Dirac cones and VHS around $A$ and $T(Y)$ points, nearly flat bands along $A-Y$ (quasi-1D band) at $-0.3$ eV below $E_F$ (blue arrows) and type-II Dirac cones along $Z-A$ and $Z-T$ paths (red arrows). The multiple (gapped) Dirac cones and VHS are common features found in kagome lattices, as already discussed in AV$_3$Sb$_5$.[15–17,27] The multiple type-II Dirac cones are unique electronic features found in double-kagome-layered CsV$_8$Sb$_{12}$, as they are absent in single-kagome-layered AV$_3$Sb$_5$. Next, we first focus on the analyses of type-II Dirac cones, which will evolve into type-II DNLs along $k_z$, leaving the discussions of VHS and quasi-1D band later.

As seen in Figure 2, type-II Dirac cones, i.e., tilted Dirac cone containing two dispersion branches with the same sign of slope, are found along both $Z-A$ and $Z-T$ lines. The Dirac energies are found $E_D = -0.2$ eV for the one along $Z-A$ and $E_D = 0$ eV for that along $Z-T$. Figure 3a shows that the bands near $E_F$ are mainly contributed by the $d$ orbitals of kagome V1 atoms and orthorhombic V2 atoms. Especially, the type-II Dirac cones along $Z-A$ are dominated by the $d$ band crossings of V2 atoms. From Figure 3a, the type-II Dirac cones also exist along $\Gamma-X$ and $\Gamma-Y$, indicating the possibility of type-II DNLs along $k_z$. To demonstrate this, we plot the 2D band structures near the band crossings with $k_z$ changed from $-\pi/c$ to $\pi/c$ in Figure 3b,c. Two groups of NLS are formed in the $k_y-k_x$ and $k_y-k_z$ planes, which include one and two lines along $k_z$, respectively. The nodal line distribution in the BZ is illustrated in Figure S1a (Supporting Information). With opposite eigenstate parities of $M_y$ ($M_x$) for these two...
crossed bands in $k_x - k_z$ space, these type-II DNLs are protected by mirror symmetry (see detailed analysis in Figure S2, Supporting Information).

It is noted that the above results are based on the calculations without SOC effect in terms of single group representation. Taking SOC into account, the DNLs will open an energy gap (<30 meV), as shown in Figure 3d and Figure S1b (Supporting Information). Considering the feature of type-II band crossing, this gap is still smaller than the energy distribution curve (EDC) width of ARPES spectra, resulting into effectively gapless features as observed. As we know, the SOC-induced Dirac gap will produce a large Berry curvature on bands crossing the Fermi level (EF). The large spin Berry curvature by NLs should yield novel spin-electronic transport behaviors, e.g., a large intrinsic spin Hall effect.

To experimentally prove the existence of these type-II DNLs, we have performed photon energy-dependent measurement. As exemplified in Figure 4a,b for spectral intensity along $Z - A$, converting the photon energy into momentum $k_z$ with an inner potential of 10 eV, clear $k_z$ periodicity can be found from the CEC in $k_z - k_x$ space at $-1.4$ eV below EF. This enables us to locate the bulk $\Gamma$ points in 3D BZ. Four $Z - A$ ARPES spectra from a series of $k_z$ values (green lines in Figure 4b and Cuts3 in Figure 4c), covering a momentum space between bulk $Z_{11}$ to $\Gamma_{12}$, are shown in Figure 4d. The Dirac energy is given in a quantitative manner by analyzing the peak positions of momentum distribution curves (MDCs) (Figure S3, Supporting Information). Red arrows in Figure 4d not only mark the effectively gapless behavior of these Dirac cones, but also their constant Dirac energies ($E_D = -0.2$ eV) along $k_z$. The existence of the type-II Dirac crossing at different $k_z$ suggests the formation of type-II DNLs. To visualize the NLs, the ARPES spectral intensity is integrated in a 0.05 eV energy window around $E_D = -0.2$ eV and plotted in $k_z - k_x$ space in Figure 4e. As marked by the white arrows, the nearly straight features along $k_z$ directly visualize these NLs formed by type-II Dirac cones along $Z - A$. Similar analyses shown in Figure 4e also demonstrate the existence of NLs around EF formed by
type-II Dirac cones along $Z - T$. Along this direction, two bands contributed by the $d$ orbitals of the V1 atoms cross twice and form two Dirac nodes (Figure 3a). At $k_z = 0$ plane, these two nodes almost merge together, while at $k_z = \pi$ plane, they are separated obviously (Figure 3c). The Dirac cone as observed in Figure 4e is supposed to be the lower half. The Dirac point moves upwards from $k_z = \pi$ plane to $k_z = 0$ plane, which is in good agreement with our DFT calculations (Figure 3c). In particular, the DNL crosses $E_F$ along $k_z$, which should play an important role in shaping the transport behavior of the material, such as the nonsaturating MR as we observed and possible large spin Hall effect.

As one of the characteristic electronic features of kagome lattice, flat bands in single-kagome-layered CsV$_3$Sb$_5$ are located beyond 1 eV below or above $E_F$ according to the DFT calculations, rendering their physical responses hardly observable. Interestingly, a low-energy flat band is observed in double-kagome-layered CsV$_8$Sb$_{12}$. To confirm the intrinsic nature of the flat band and exclude the nondispersive core level spectra excited by twice the photon energy, it is necessary to examine whether the binding energy position of the flat band changes with the photon energy. As shown in Figure 5a,b, our ARPES spectra with both photon energies of 80 and 79 eV demonstrate a nearly nondispersive band along the BZ boundary $A - Y - A'$ at $\sim$-0.4 eV below $E_F$. The excitation energy independence of this band eliminates the possibility of core level spectra excited by twice the photon energy and reveals its intrinsic nature. The DFT calculated band structure along the same high-symmetry path is shown in Figure 5c, which is in good agreement with the ARPES measurements. Obviously, a weakly dispersive band is present along $A - Y - A'$ but absent along other paths, e.g., along $Y - Z$ or $Z - T$ as shown in Figure 5e or 3a, indicating its quasi-1D behaviors. Our DFT calculations further reveal that this quasi-1D band is contributed by the $d$ orbitals of kagome V1 atoms. However, it is different from the usual flat band in the kagome lattice which arises from a destructive phase interference of hopping. To visualize the origin of this quasi-1D band, we plot the wave function of its electronic states in Figure 5d. Instead of uniformly distributing on three V atoms in the kagome lattice, the electronic states of quasi-1D band are mainly located at one V atom. The wave functions hybridize with the adjacent ones to form an approximate striped distribution. In addition, the $p$ orbitals of Sb atoms from orthorhombic V$_2$Sb$_2$ layer also have small contributions to the hybridizations of these states (Figure S4, Supporting Information).

VHSs, another typical feature of kagome lattice, are also found in this double-kagome-layered system. As shown in Figure 5e, near $E_F$, DFT predicts two VHSs at $Y$ (VHS1) and $\Gamma$ (VHS2), respectively. Remarkably, the VHS2 at $\Gamma$ lies slightly above $E_F$ (Figure 5f), temptingly calls for electron doping to manifest its physical response. It is noted that this VHS originates from the orthorhombic V$_2$Sb$_2$ layer rather than the kagome lattice (Figure 3a). Considering that the VHS usually exists at BZ boundary in kagome lattice, the VHS2 at BZ center is scarce and deserves further investigation. VHS1 at $Y$, $\sim$-0.3 eV below $E_F$, is directly observed in ARPES spectra (Figure 5g,h). More interestingly, it almost has the same binding energy with the quasi-1D band and they interact with each other at $Y$, as illustrated in the inset of Figure 5e. Since both quasi-1D and VHS feature enhanced density of states, as directly visualized by the very high intensity in Figure 5g,h, their low-energy nature calls for topological and correlated electron transport experiments via local electrostatic gates. Compared to CsV$_3$Sb$_5$, the two VHSs are located above or below the Fermi level in CsV$_8$Sb$_{12}$, probably accounting for the vanishing of CDW in the double-kagome-layered CsV$_8$Sb$_{12}$,
which may further reflect the important role of VHS position in the formation of CDW in V-based kagome materials.[42]

3. Conclusion

Combining experimental and calculational analyses, we have performed systematic investigations on the electronic structure of double-kagome-layered CsV₈Sb₁₂. We have revealed unique electronic features in this compound, including multipletype-II DNLs as well as interacted quasi-1D band and VHS. The non saturating MR behavior we have observed may originate from the coexistence of electron and hole Fermi pockets induced by the type-II Dirac cones. Being a great cousin for comparative study of CsV₃Sb₅, our results prove CsV₈Sb₁₂ as an ideal platform to investigate the distinct properties of these novel electronic features. The type-II DNLs, especially the one lying at the Fermi level, should play a significant role in shaping the transport response of the material and deserve further theoretical and experimental study. The zone-center VHS and enhanced spectral weight featured by interacted quasi-1D band and VHS stimulate local electrostatic control for topological and correlated electronic physics.

4. Experimental Section

Sample Growth and Characterization: High-quality CsV₈Sb₁₂ single crystals were grown by self-flux method. High-purity Cs (clump), V (powder), and Sb (ball) were mixed with a ratio of 1:6:18 in the glove-box and placed into an alumina crucible. The crucible was then double-sealed into the evacuated quartz tubes to prevent the quartz tube from being corroded by Cs during heating. The assembly was first heated very slowly to 500 °C and kept for 5 h. Then the furnace was raised to 1100 °C and held at this temperature for another 24 h for proper homogenization. Finally, the furnace was cooled down to 900 °C at a rate of 1 °C h⁻¹. The crystals were separated from the flux by centrifuging. The structure of the crystals was determined by X-ray diffraction with Cu Kα radiation at room temperature using a Rigaku MiniFlex diffractometer.

ARPES Measurement: ARPES measurements were performed at the BL03U beamline of the Shanghai Synchrotron Radiation Facility (SSRF) and beamline 13U of the National Synchrotron Radiation Laboratory (NSRL). The energy resolution was set at 15 meV for Fermi surface mapping and 7.5 meV for band structure measurements. The angular resolution was set at 0.1°. Samples were cleaved in situ under ultrahigh vacuum conditions with pressure better than 5 × 10⁻¹¹ mbar and temperatures below 20 K.

First-Principles Calculations: The first-principles calculations were performed using the Vienna ab initio simulation package[43] within the projector augmented wave method[44] and the generalized gradient approximation of the Perdew–Burke–Ernzerhof[45] exchange-correlation functional. The plane-wave basis with an energy cutoff of 400 eV, the experimental lattice constants of a = b = 5.495 Å and c = 9.308 Å, and the Γ-centered 9 × 9 × 9 k-point meshes are adopted. The spin-polarized calculations are tested, which give a nonmagnetic ground state. The SOC effect is also considered in part of the calculations. A tight-binding (TB) Hamiltonian based on the maximally localized Wannier functions (MLWF)[46] is constructed to get the energy eigenvalues and eigenstates for further Fermi surface plot using the WannierTools package.[47] Using MLWF, the spin Berry curvature for the nth band at k is
calculated by

\[ \Omega_{\alpha\beta}^n(k) = -\sum_{n'\neq n} \frac{2im}{(e_{kn} - e_{kn'})^2} \langle \mathbf{k} n | j_\alpha \mathbf{p} | \mathbf{k} n' \rangle \langle \mathbf{k} n' | j_\beta \mathbf{p} | \mathbf{k} n \rangle \]  

(1)

Here, \( j_\alpha = \hat{x}_\alpha, \hat{y}_\alpha/2 \) is the spin current operator, \( \alpha \) and \( \beta \) denote the three Cartesian directions \( x, y, \) and \( z, j_\alpha = (\hbar/2) \hat{\Sigma}_\alpha \), where \( \Sigma \) is a 4 x 4 matrix and \( \Sigma \) is the spin operator in the Dirac equation, and \( | \mathbf{k} n \rangle \) represents the periodic part of the Bloch wave function with energy \( e_{kn} \).

Supporting Information

Supporting Information is available from the Wiley Online Library or from the author.

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Conflict of Interest

The authors report no conflict of interest.

Data Availability Statement

The data that support the findings of this study are available from the corresponding author upon reasonable request.

Keywords

nonsaturating magnetoresistance, quasi-1D band, spin Berry curvature, type-II Dirac nodal line semimetal, van Hove singularity
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