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Electronic states in superconducting type-II Dirac semimetal: 1T-PdSeTe

Yogendra Kumar[1], Shiv Kumar[2], Yenugonda Venkateswara[3,4], Ryohei Oishi[1], Jayata Nayak[4], R.P. Singh [6], Takahiro Onimaru[1], Yasuyuki Shimura [1], Chaoyu Chen[5], Shinichiro Ideta[2], Kenya Shimada[2,7,8]

[1]*Graduate School of Advanced Science and Engineering, Hiroshima University, Higashi-Hiroshima 739-8526, Japan*
[2]*Research Institute for Synchrotron Radiation Science (HiSOR), Hiroshima University, Higashi-Hiroshima 739-0046, Japan*
[3]*Department of Physics, SUNY Buffalo State University, Buffalo, New York 14222, USA*
[4]*Department of Physics, Indian Institute of Technology, Kanpur 208016, India*
[5]*Songshan Lake Materials Laboratory, Dongguan 523808, China*
[6]*Department of Physics, Indian Institute of Science Education and Research, Bhopal 462066, India*
[7]*The International Institute for Sustainability with Knotted Chiral Meta Matter (WPI-SKCM2), Hiroshima University, Higashi-Hiroshima 739-8526, Japan*
[8]*Research Institute for Semiconductor Engineering (RISE), Hiroshima University, Higashi-Hiroshima 739-8527, Japan*

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Recently topological semimetals have attracted much interest for their non-trivial band structures [1-3] that can be categorized into Dirac semimetals (DSMs), Weyl semimetals (WSMs), and topological nodal-line semimetals based on their band crossing characteristics near the Fermi level [4]. Layered transition metal chalcogenides, found among DSMs and WSMs, are notable for their diverse physical properties like superconductivity and charge density wave (CDW), with promising applications [5].

We synthesized high-quality single crystals of the superconducting type-II Dirac semimetal 1T-PdSeTe using a two-step melting method and characterized their crystal quality via XRD, EPMA, and cross-sectional S-TEM with EDX. Scanning transmission electron microscopy confirmed a homogeneously mixed Se/Te distribution within the CdI_2-type lattice. Angle-resolved photoemission spectroscopy (ARPES) at HiSOR BL-1 and UVSOR BL5U beamlines, along with density functional theory (DFT) calculations using ordered/disordered supercell and slab models, revealed topological surface states, a surface Dirac cone, and a type-II bulk Dirac-like crossing along the Γ–A direction.

Compared to 1T-$PdTe_2$ (T_c = 1.6 K), PdSeTe exhibited an enhanced superconducting transition temperature (T_c = 3.2 K), likely due to chemical pressure effects rather than atomic disorder. The persistence of electronic band dispersion and local structures upon substitution suggests that the CdI_2-type lattice symmetry governs the band structure. These findings provide insights into the role of solid solutions in modifying surface and bulk electronic states and enhancing superconductivity in Dirac semimetals.

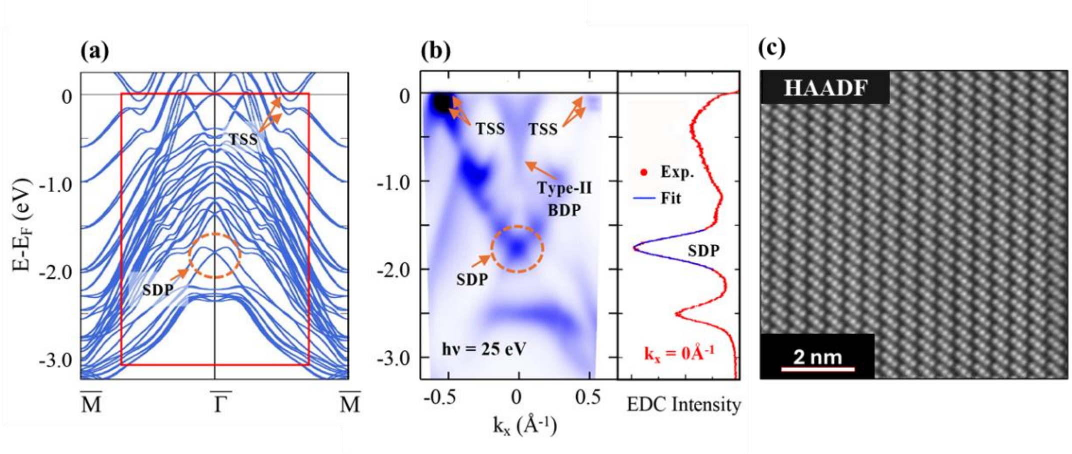

Fig. 1: (a) and (b) represent the simulated bands for slab (5 atomic layers) and measured ARPES spectrum along $\overline{\mathrm{M}} - \overline{\Gamma} - \overline{\mathrm{M}}$ direction with 25eV photon energy at 20K, respectively. (c) High-resolution STEM, High angle annular dark field (HAADF) image of the (100) plane of a 1T-PdSeTe crystal.

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