Doping-Induced Evolution of the Electronic Band Structure in Ni-Doped PdSeTe

Yogendra Kumar[1], Takahiro Onimaru[2], Yasuyuki Shimura [2], Shinichiro Ideta[1], Kenya Shimada[1]

[1]*Research Institute for Synchrotron Radiation Science (HiSOR), Hiroshima University, Higashi-Hiroshima 739-0046, Japan*
[2]*Graduate School of Advanced Science and Engineering, Hiroshima University, Higashi-Hiroshima 739-8526, Japan*

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The interplay between superconductivity and topology in 111-type transition-metal dichalcogenides (TMDCs) provides a promising platform for realizing topological superconductivity [4-6]. PdSeTe exhibits enhanced superconductivity (Tc ≈ 3.2 K) [1] while preserving topological surface states. In contrast, partial substitution of Pd with Ni completely suppresses superconductivity, despite nearly identical crystal symmetry and overall band dispersion. This striking contrast offers a unique opportunity to isolate the microscopic ingredients governing superconductivity.

In this study, we investigate the doping-induced evolution of the electronic structure in Ni-doped PdSeTe using high-resolution synchrotron ARPES and first-principles calculations that include spin-orbit coupling. Our measurements reveal that, although the global band topology and Dirac-like surface states remain robust under Ni substitution, subtle yet critical modifications occur in the orbital character and Fermi-surface topology. Density functional theory (DFT) calculations indicate that replacing Pd 4d orbitals with more localized Ni 3d orbitals modifies hybridization strength and effective spin-orbit coupling, thereby redistributing spectral weight near the Fermi level.

These results demonstrate that superconductivity in PdSeTe is highly sensitive to transition-metal orbital character rather than lattice symmetry alone. Our findings establish Ni substitution as a powerful tuning parameter for disentangling orbital, spin-orbit, and lattice contributions, and provide key insights into the microscopic conditions required for superconductivity in topological TMDCs.

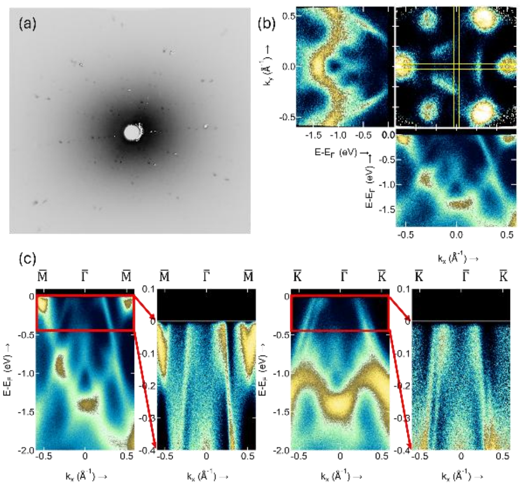

FIGURE 1. (a-c) Laue and *ARPES measurements on Ni-doped PdSeTe confirm the lattice symmetry and topological surface states similar to PdSeTe.*

REFERENCES

[1]. **Y. Kumar et al.**, *Enhanced Superconductivity with Preserved Topological States in PdSeTe*, **Phys. Rev. Research 7**, 013174 (2025).
[2]. **H.-J. Noh et al.**, *Experimental Realization of Type-II Dirac Fermions in $PdTe_2$*, **Phys. Rev. Lett. 119**, 016401 (2017).
[3]. **P. K. Das et al.**, *Bulk superconductivity in type-II Dirac semimetal $PdTe_2$*, **Phys. Rev. B 97**, 014523 (2018).
[4]. **M. Z. Hasan and C. L. Kane**, *Colloquium: Topological insulators*, **Rev. Mod. Phys. 82**, 3045 (2010).
[5]. **N. P. Armitage, E. J. Mele, and A. Vishwanath**, *Weyl and Dirac semimetals in three-dimensional solids*, **Rev. Mod. Phys. 90**, 015001 (2018).
[6]. **M. Sato and Y. Ando**, *Topological superconductors: a review*, **Rep. Prog. Phys. 80**, 076501 (2017).