DOCTORAL DISSERTATION: ABSTRACT

EXPLORING ELECTRONIC PROPERTIES OF TOPOLOGICAL SEMIMETALS TaAs₂ AND NbP: CRYSTAL GROWTH, ELECTRON TRANSPORT AND ARPES STUDIES

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ABSTRACT

In this PhD thesis, we investigated the electronic properties of two topological semimetals, TaAs₂ and NbP. Electron transport and angle-resolved photoemission spectroscopy (ARPES) measurements were performed on TaAs₂ single crystals on (201) surface. Fourier analysis of the Shubnikov-de Haas oscillations revealed four distinct peaks and their angular dependence was examined relative to the magnetic field orientation. The results indicate elliptical Fermi surface cross-sections. Mobility spectrum analysis confirmed the presence of at least four types of carriers contributing to the conductance at 1.6 K, including two types of electrons and two types of holes. ARPES spectra on the freshly cleaved $(\overline{201})$ surface confirmed the elliptical shape of the bulk states pockets, supporting the magnetotransport angle-dependent studies. With an increased Fermi level due to weak n-doping, theoretical calculations reproduced the ARPES data better. The studies facilitated the understanding of the physics of Dirac and Weyl points in this compound. Furthermore, we performed ARPES studies to examine Fermi surface modifications in NbP semimetal with in-situ deposition of ultra-thin layers of Pb and Nb. Pristine single crystals with P and Nb terminations of the (0 0 1) surface were investigated. The P-terminated surface exhibited spoon and bow-tie-shaped surface states, while the Nb-terminated surface lacked these features. Deposition of a single monolayer (ML) of Pb induced a topological Lifshitz transition (TLT) in P-terminated NbP, exchanging the pair of Weyl points connecting adjacent Brillouin zones. The Fermi surface was modified along with a shift in the Fermi energy. On the other hand, the deposition of approximately 0.8 ML of Nb pushed the electronic structure of P-terminated NbP close to the critical point of a TLT, partial transformation. Despite the Fermi surface evolution, surface Fermi arcs remained connected to topologically protected Weyl points. Additionally, Nbterminated NbP covered with 1.9 ML of Pb exhibited altered trivial surface states caused by Lifshitz transition.

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