

Surface density of states in Pt_2HgSe_3 investigated by quasiparticle interference

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Jacutingaite, with chemical formula Pt_2HgSe_3 , is a layered material that in bulk form manifests a dual topological character by hosting a weak topological phase and a mirror-protected topological crystalline phase. This topological duality has been investigated theoretically [1, 2] and experimentally by high-resolution angle-resolved photoemission spectroscopy (ARPES) [3]. Here, we extend the experimental investigation to the conduction band—not accessible by ARPES—by means of scanning tunneling spectroscopy (STS), Fourier transform STS, and density functional theory (DFT) calculations. The experiments have been performed at low temperatures and in UHV on high quality single crystals grown at the DQMP. Despite its semimetallic character, at high junction resistances (R_J) the spectroscopy curves appear insulating with a large gap ~ 0.8 eV, while they have metallic behavior in the limit of low R_J . Our DFT calculations explain this behavior with a reconstruction of the surface crystal structure leading to insulating behavior at the topmost layer. We identify several robust spectroscopic features in the density of states in both the conduction and valence band. Quasiparticle interference allows to track their origin to the existence of surface states. We discuss the observed dispersive character and the possible topological nature with the support of DFT calculations.

[1] Marrazzo, A., N. Marzari, and M. Gibertini, *Emergent dual topology in the three-dimensional Kane-Mele Pt_2HgSe_3* . Physical Review Research, 2020. **2**(1).

[2] Facio, J.I., et al., *Dual topology in jacutingaite Pt_2HgSe_3* . Physical Review Materials, 2019. **3**(7).

[3] Cucchi, I., et al., *Bulk and Surface Electronic Structure of the Dual-Topology Semimetal Pt_2HgSe_3* . Phys Rev Lett, 2020. **124**(10): p. 106402.