Charge dynamics in the Weyl semimetals $NbIrTe_4$ and $TaIrTe_4$ under pressure: Signatures of an electronic phase transition

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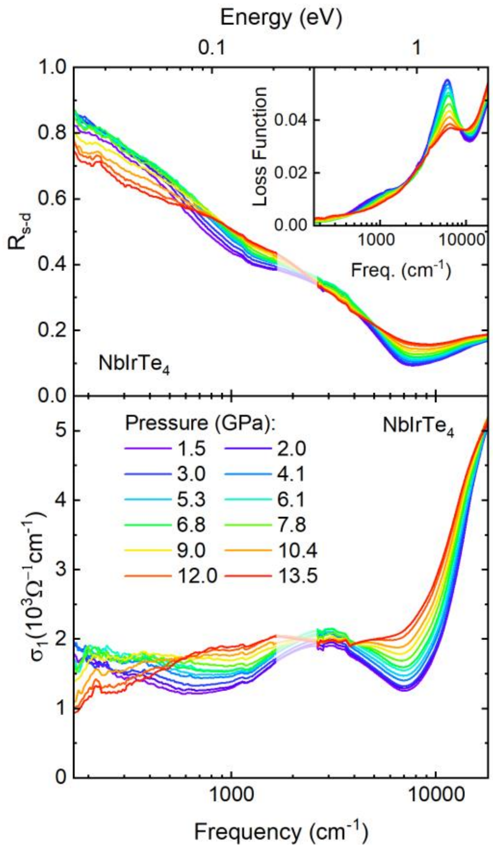
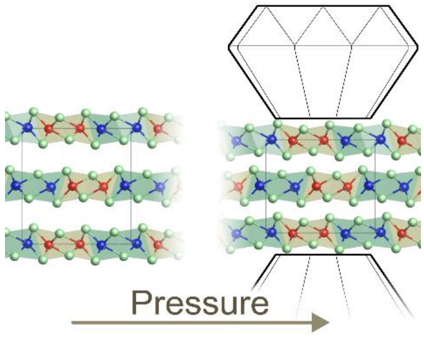
Abstract

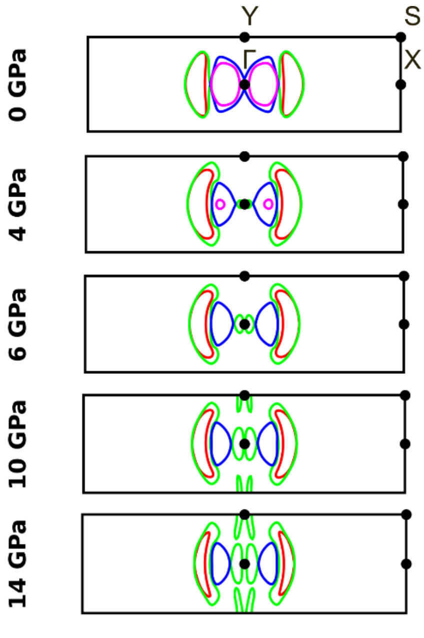
The ternary transition-metal iridium tellurides $NbIrTe_4$ and $TaIrTe_4$ are proposed as type-II Weyl semimetals. Applying external hydrostatic pressure is an effective method for tuning their electronic and structural properties. In this study, we present a high-pressure investigation of the charge dynamics in $NbIrTe_4$ and $TaIrTe_4$ using infrared spectroscopy supplemented by density functional theory calculations. Our experimental optical conductivity spectra reveal a clear phase transition occurring at a critical pressure of 7-8 GPa in both compounds. Above this critical pressure, we observe a significant redistribution of spectral weight in the optical conductivity spectrum. A Drude-Lorentz analysis indicates a sharp reduction in the free carrier concentration. Consequently, a previously obscured low-energy phonon mode emerges as a distinct feature, because the screening effect from the Drude contribution is weakened. Raman scattering measurements show no evidence of a significant structural phase transition, suggesting that the observed anomalies are predominantly electronic in nature. Our ab initio calculations support this conclusion; they indicate that the total density of states at the Fermi level remains remarkably constant. Instead, the reduction in Drude weight is driven by significant topological modifications of the Fermi surface, specifically the shrinking and fragmentation of electron and hole pockets. These purely electronic transitions involving topological changes to the Fermi surface are characteristic of a Lifshitz transition. Ultimately, these results provide collective evidence for a pressure-induced, Lifshitz-type electronic phase transition driven by tuned van der Waals interlayer coupling.



Evolution of the reflectivity and optical conductivity in $NbIrTe_4$ under pressure. The transition at P_c = 7-8 GPa is evidenced by a sharp decrease in Drude weight alongside an increase in interband transitions.



Schematic illustration of the high-pressure evolution. The application of hydrostatic pressure via a diamond anvil cell primarily compresses the soft van der Waals gap, leading to a significant decrease in the interlayer distance along the c-axis.



Evolution of the Fermi surface cross-sections of $NbIrTe_4$ under hydrostatic pressure.