High-energy excitations in the type-II Dirac semimetal $PtTe_2$

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Recently, the PtX_2 (X = Se, Te, S) class of transition metal dichalcogenides (TMDCs) has attracted considerable interest as one of the most promising among layered materials "beyond graphene".
The enormous effort directed toward the PtX_2 class is motivated by the existence of bulk type-II Dirac fermions, arising from a tilted Dirac cone [1,2].
Thin layers of the PtX_2 class of materials are evenly interesting because of their relatively high mobility that combined with energy-gap tunability upon thickness reduction might enable the fabrication of field-effect transistors to be employed in optoelectronics [3] and gas sensing [4].
Although the band structure of $PtTe_2$ has been explored comprehensively, along with the Dirac plasmons (collective density excitations) in the infrared range of the electromagnetic spectrum [5], the high-energy excitations in $PtTe_2$ still remain unexplored.
Here, we explore the broadband excitation spectrum of bulk crystals and thin layers of $PtTe_2$, using electron energy-loss spectroscopy (EELS) in reflection mode for bulk and EELS in combination with scanning transmission electron microscopy (STEM-EELS) for thin layers.
In the case of bulk $PtTe_2$, we observe modes at 3.9, 7.5, and 19.0 eV in the ultraviolet region, in addition to infrared modes related to intraband three-dimensional (3D) Dirac plasmon and interband transitions between the 3D Dirac bands. These observations are well explained by the density-functional theory(DFT)-based orbital-resolved band-structure and orbital-resolved density of states(DOS) calculations. We find that in bulk $PtTe_2$ the observed peaks at 3.9, 7.5, and 19.0 eV are predominantly connected to $Pt_{5d} \rightarrow Pt_{5d}$, $Te_{5p} \rightarrow Te_{5d}$, and $Te_{5s} \rightarrow Te_{5d}$ transitions, respectively. In thin layers, with decreasing thickness, we show that, unlike graphene, the high-energy EELS peak in $PtTe_2$ thin film gets redshifted by ~ 2.5 eV with increasing thickness.
These informations on the excitation spectrum of collective modes in the visible-ultraviolet range represent an essential step to devise broadband photodetectors, ultraviolet-imaging applications, and broadband plasmonic devices.

References

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