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Tantalum phosphide: A topological weyl semimetal.

Topological semi-metals are newly discovered states of quantum matter that have arose interest in the research community due to their application in spintronics and valleytronics. There are three types of topological semi-metals (TSMs); Dirac Semi-metal (DSM), Weyl Semi-metal (WSM) and Node Line Semi-metal (NLSM), each with special features that makes them novel candidates for future technologies. Unlike topological insulators (TI) that have an energy gap, TSMs have their valence and conduction bands touching in discrete points in the Brillouin zone. Tantalum phosphide (TaP), has been classified as a weyl semi-metal with only a single type of Weyl fermions and thus topologically distinguished from tantalum arsenide (TaAs) that has two types of Weyl fermions. Theoretically, if spin-orbit interaction is turned on in the system, we expect an energy gap. To this date, little has been devoted on this relativistic interaction in TaP. Our goal will be to calculate the bandstructure in TaP and how the spin-orbit interaction alters the single Weyl fermions. We will employ first-principles density functional theory (FPDFT) as implemented in SIESTA code. This study is not only based on fundamental research interests but also of great potential for future applications.

Keywords

TSMs, WSM, first-principles, Density functional theory.

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