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Unique topological nodal line states and associated exceptional thermoelectric power factor platform in Nb_3GeTe_6 monolayer and bulk†

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To date, ideal topological nodal line semimetal (TNLS) candidates in high dynamically stable and high thermally stable two-dimensional (2D) materials are still extremely scarce. Herein, by performing first-principles calculations, on the one hand, we found that three-dimensional Nb_3GeTe_6 bulk possesses a single closed TNL in the k_x = 0 plane and a fourfold TNL in the S–R direction without considering spin–orbit coupling (SOC). Under the SOC effect, a new topological signature, *i.e.*, hourglass-like Dirac nodal line, occurs in Nb_3GeTe_6 bulk. On the other hand, we found that the 2D Nb_3GeTe_6 monolayer features a doubly degenerate TNL along surface X–S paths. Importantly, this monolayer enjoys the following advantages: (i) it has high thermal stability at room temperature and above; (ii) its TNL is nearly flat in energy and is very close to the Fermi level (E_F), which provides a fantastic maximum value platform of the thermoelectric power factor around the E_F; and (iii) no extraneous bands are close to the TNL, near the Fermi level. Moreover, we explore the entanglement between the topological states and thermolectric properties for the 2D Nb_3GeTe_6 monolayer. Our work not only reports the discovery of a novel TNL material, but also builds the link between the TNL and thermoelectric properties.

1. Introduction

Based on their electronic structures, materials may feature non-trivial band topologies.[1] The exploration of this non-trivial band topology has led to a new field, *i.e.*, topological materials, and this field has attracted widespread attention from researchers in physics, chemistry, and materials science. Initially, the investigations in this area were mainly focused on insulating materials,[2–10] but recent research has expanded from insulators to metallic and semimetallic materials.[11–47] Three-dimensional (3D) topological semimetallic materials (TSMs) can be roughly classified into three types: (i) topological nodal point semimetals (TNPSs),[3,18,20,23,26,32,34] such as Dirac-point semimetals (DPSs)[13,20,32,34] and Weyl-point semimetals (WPSs);[18,23] (ii) topological nodal line semimetals (TNLSs);[16,17,24,36] and (iii) topological nodal surface semimetals (TNSSs).[41,45–47] In these TSMs, the topology is strongly associated with low-energy non-trivial band crossing points (BCPs). For example, in Weyl semimetals,[23] the conduction band (CB) and the valence band (VB) intersect at isolated nodal points. Around these zero-dimensional (0D) isolated nodal points, the dispersions of the bands are linear in all directions, and the low-energy electrons behave similarly to Weyl fermions in high-energy physics. A series of materials have been proposed as candidates for TNPSs *via* first principles calculations, and among them, some well-known materials, including Cd_3As_2,[20,42] Na_3Bi,[34,43] and the TaAs[44] family, were experimentally confirmed.

The TNLSs possess band crossing points (BCPs) along a line[11,24,32,36,40] with a one-dimensional (1D) topological element. To date, many interesting forms of behavior have been observed among the TNLSs, including a topological surface state,[48,49] anisotropic non-saturating magetoresistance,[50] and possible high temperature superconductivity.[51] Many materials with different 1D topological elements[52–55] have been predicted based on first principles and some of them, such as $PbTaSe_2$[56] and metallic-mesh photonic

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