Novel Topological Magnetic Insulators in Transition-Metal Trichalcogenides

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Recently, there has been active research development in two-dimensional materials beyond graphene, which consist of transition-metal chalcogenides and halides in potential applications for field-effect transistors, spintronics and valleytronics, thermoelectrics, and topological insulators. Here we show that the two-dimensional materials consisting of transition-metal chalcogenides, e.g., transition-metal trichalcogenides (TMTC), have interesting features in their electronic band structure, which lead to novel magnetic interactions and topological characteristics like Chern insulators. From density-functional-theory calculations, we demonstrate that a class of TMTC compounds becomes a ferromagnetic insulator with a non-trivial Chern number. While transition metal atoms are responsible for the ferromagnetic ground state, the band topology depends on the hopping matrix elements through chalcogen atoms. The nontrivial band topology is confirmed to have a nonzero Chern number, quantized Hall conductivity, and chiral edge states by using the Wannier function analysis. We propose the strong dpσ hybridization as a new channel of magnetic interactions in TMTC materials. Further prospects of Chern insulator materials will be discussed.

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