From Pentagonal Geometries to Two-Dimensional Materials

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The Cairo tessellation refers to a pattern of type 2 pentagons that can pave an infinite plane without creating a gap or overlap. We reveal the hidden, layered Cairo tessellations in the pyrite structure with a general chemical formula of AB_2 and space group pa$\overline{3}$. We use this hidden tessellation along with density functional calculations to examine the possibility of obtaining a two-dimensional (2D) material with the Cairo tessellation from the bulk, using PtP_2 as an example. Unlike previously reported single-layer materials such as $PdSe_2$ with a buckled, pentagonal structure— strictly speaking, not belonging to the Cairo tessellation, we find that single-layer PtP_2 is completely planar exhibiting dynamically stable phonon modes. We also observe a reduction in the bandgaps PtP_2 from bulk to single layer using the Heyd-Scuseria-Ernzerhof (HSE) hybrid density functional, and the bandgap type switches from indirect to direct. By contrast, using the standard Perdew-Burke-Ernzerhof functional leads to the conclusion of single-layer PtP_2 being metallic. We further study the bonding characteristics of this novel single-layer material by computing the Bader charge transfer, the electron localization function, and the crystal orbit overlap population, which show mixed P-P covalent bonding and Pt-P ionic bonding, with the former being stronger. Finally, we study the surface states of single-layer PtP_2 and consider the spin-orbit coupling. We observe no spin-helical Dirac cone states, therefore ruling out single-layer PtP_2 as a topological insulator. We expect the example demonstrated in this work will stimulate interest in computationally identifying novel 2D materials from a variety of bulk materials with the pyrite structure.

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