Nontrivial Topology in Monolayer MA_2Z_4 (M = Ti, Zr, or Hf; A = Si or Ge; and Z = N, P, As, Sb, or Bi)

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Abstract

The search for two-dimensional (2D) materials with interesting topological properties is still attracting growing interest as they offer exotic physical phenomena. Recently, the emergent 2D MA_2Z_4 has been gaining attention because it exhibits versatile properties due to its tunable elemental components M, A, and Z. In this study, an exhaustive search coupled with first-principles calculations was performed to investigate 30 MA_2Z_4 (M is Group IV transition metals Ti, Zr, or Hf; A is Si or Ge; and Z is pnictogens N, P, As, Sb, or Bi) monolayers under two crystal phases called T-phase and H-phase, totaling to 60 structures. Ground state energy calculations revealed that all materials energetically prefer the T-phase. Remarkably, Z_2 topological invariant calculated under hybrid functional HSE06 reveals five MA_2Z_4 monolayers ($TiSi_2Bi_4$, $ZrGe_2P_4$, $ZrGe_2As_4$, $HfSi_2As_4$, and $HfGe_2As_4$) to have nontrivial topology. This topological phase transition was driven by the spin-orbit coupling resulting in the splitting of the d_{z^2} orbital of transition metal elements and $p_x + p_y$ orbitals of pnictogen elements. The nontrivial properties were further confirmed by the presence of gapless edge states. Phonon spectra and ab initio molecular dynamics verified that all nontrivial materials are thermodynamically stable. Our results indicate that the new MA_2Z_4 family has fascinating properties and possesses strong potential for applications in electronics and topological devices, which will stimulate interest in experimental synthesis.