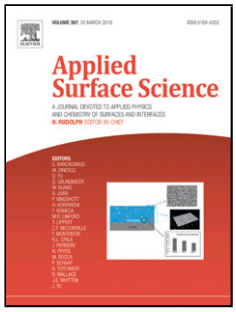

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Electronic Structure and Topological Features of Tin-based Binary Nanosheets and Their Hydrogenated/Fluorinated Derivatives: A First-principles Study

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Abstract

Utilizing first-principles calculations, we have investigated the structural, electronic and topological properties of binary SnSi and SnGe nanosheets as well as their H-/F- derivatives. It is found that all these systems have chair-like buckled configurations with robust structural stabilities. Unlike the elemental group-IV sheets, SnSi and SnGe sheets are narrow-band-gap semiconductors, which have a gapped Dirac cone with massive Fermions. Under the strains, a direct-to-indirect band gap transition and a semiconductor-to-metal transition would occur in these systems. Although these binary systems are trivial band insulators with $\mathbb{Z}_2$=0, their topological features can be altered by the surface decorations. Particularly, the fluorinated SiGe sheet becomes a topological insulator with $\mathbb{Z}_2$=1, and such non-trivial state can also be found in the strained fluorinated SnSi and hydrogenated SnGe sheets. Large non-trivial SOC band gaps of 0.09−0.17 eV are obtained in these 2D topological insulating systems, which will be beneficial for realizing the room-temperature quantum spin Hall effect. Our study demonstrates

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