Zhongqin YANG'S Group

From Nodal-line Semimetals to Topological Insulators in Two-dimensional halogenated tetragonal stanene SnX (X = F, Cl, Br, I)

Ye Zhu, Wenting Xu, Wei Xu, Hongyan Zhao, Yang Xue, and Zhongqin Yang*

State Key Laboratory of Surface Physics, Key Laboratory for Computational Physical Sciences (MOE) and Department of Physics, Fudan University, Shanghai 200433, China

Abstract

Based on first-principles calculations, we explore a new family of two-dimensional (2D) halogenated tetragonal stanene SnX (X = F, Cl, Br, I) monolayers. The various decorating halogens are found facilitating the mutual transformation between 2D nodal-line semimetals (NLSMs) and 2D topological insulators (TIs) in the tetragonal SnX (T-SnX) monolayers with X = F, Cl, Br, I. Due to the different strengths of spin-orbit coupling (SOC), the T-SnF and T-SnCl monolayers are nodal-line semimetals while the T-SnBr and T-SnI are topological insulators. The nodal-line characteristic in T-SnF and T-SnCl is justified by three-dimensional (3D) band structure around the Γ point. The quantum spin Hall (QSH) states in the T-SnBr and T-SnI are identified by a single pair of topologically protected helical edge states locating inside the bulk gap as well as a nontrivial topological invariant $Z_2 = 1$. The unique electronic states in 2D T-SnX monolayers render them to become a highly promising material platform for the development of innovative electronic devices.

Geometry structures

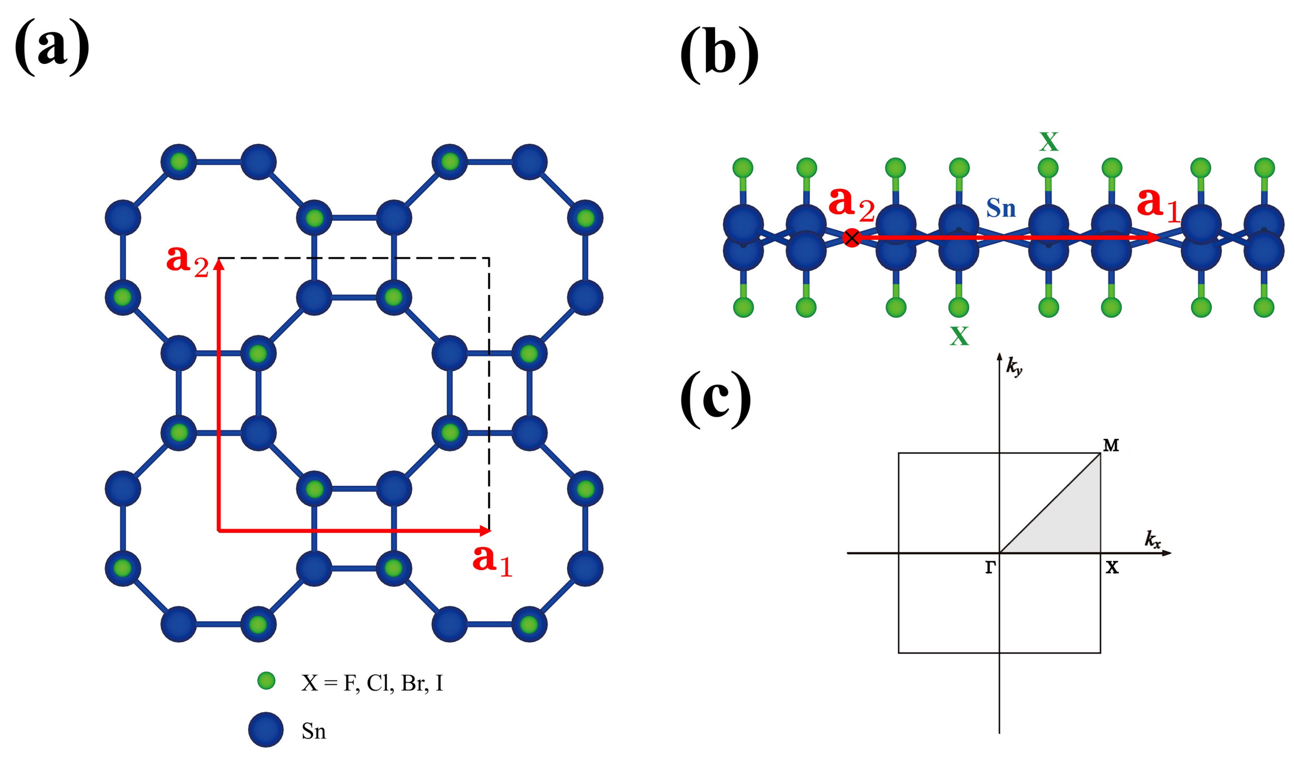

FIG. 1. Top (a) and side (b) views of the schematic structures of T-SnX monolayer with Bravais lattice vectors $\mathbf{a}_1$ and $\mathbf{a}_2$. Blue and green balls denote Sn and X (X = F, Cl, Br, I) atoms, respectively. (c) The first Brillouin zones of the T-SnX monolayers.

Electronic structures

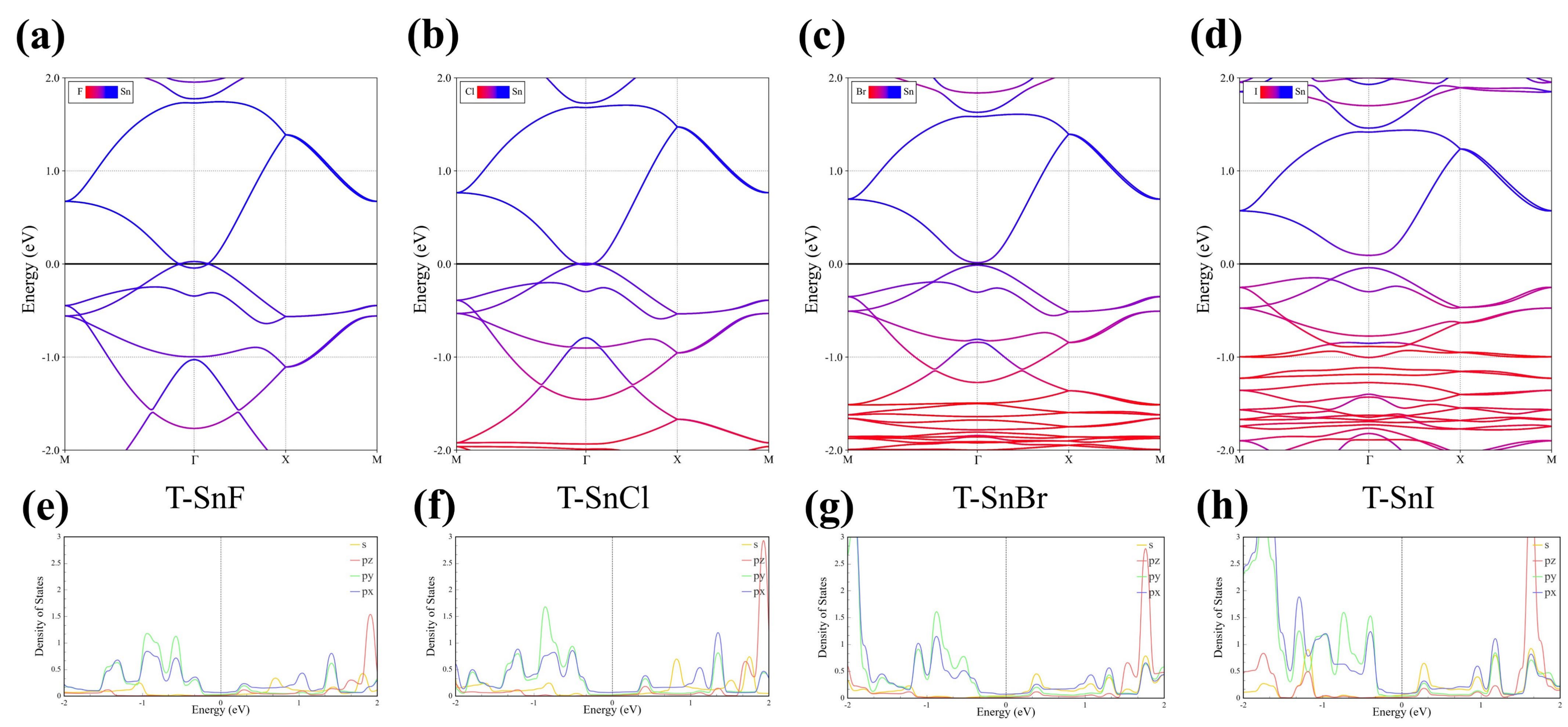

FIG. 2. The band structures (upper row) and PDOS (lower row) for (a,e) T-SnF, (b,f) T-SnCl, (c,g) T-SnBr, (d,h) T-SnI monolayers with SOC.

Nodal-line Semimetals

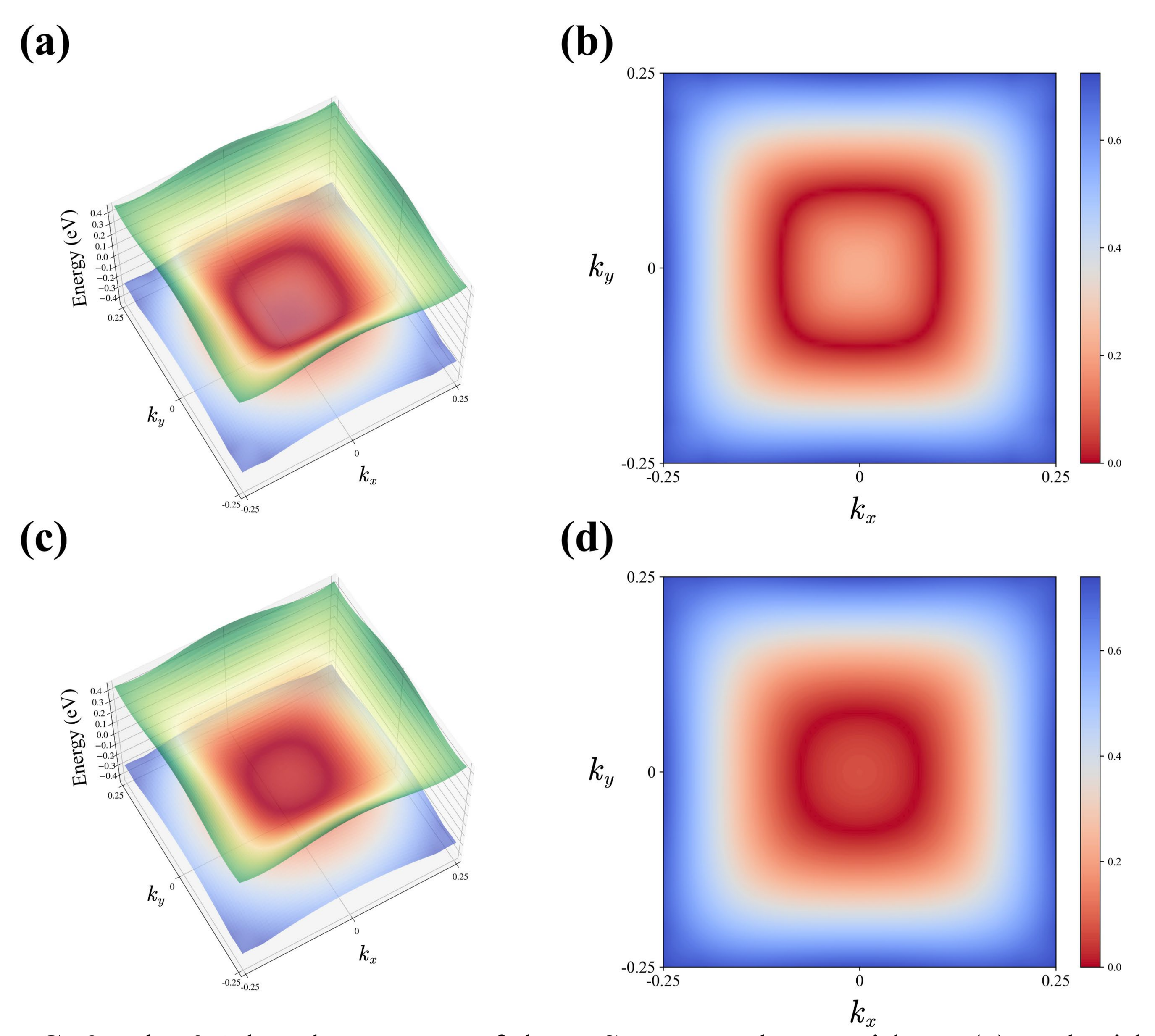

FIG. 3. The 3D band structure of the T-SnF monolayer without (a) and with (c) SOC around the Γ point. A closed red line is seen in each structure, indicating unique nodal-line bands obtained. The heat maps (b) and (d) reflect the absolute values of the difference between the corresponding conduction and valence bands.

Topological Insulators

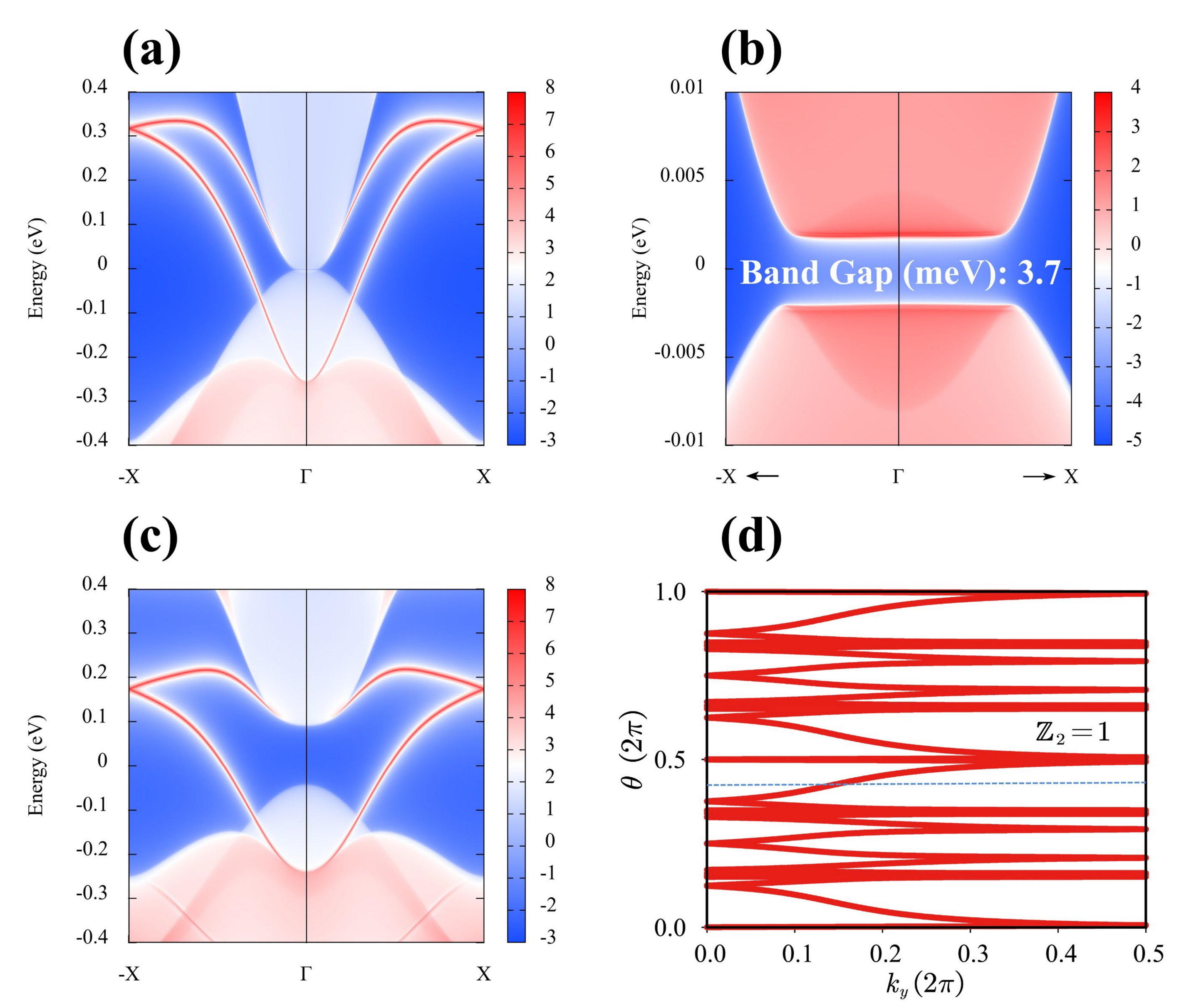

FIG. 4. Topological edge states of T-SnCl (a) and T-SnI (c) monolayers with SOC. The Fermi level is set to zero. (b) The enlarged view near the Fermi level demonstrates a 3.7 meV band gap in the T-SnCl monolayer. (d) Evolution of the Wannier charge center (WCC) along ky at kz = 0 plane in Brillouin zone of the T-SnI nanosheet.

Conclusions

- The nodal-line band structures are realized exactly at the Fermi level in the T-SnX (X=F, Cl, Br, I) monolayers without SOC due to the protection of the glide mirror. While the tiny global topological nontrivial band gaps (less than 5 meV) occur in T-SnF and T-SnCl monolayers with SOC, they can still be regarded as nodal-line semimetals due to the small band gaps.
- The global topological nontrivial band gaps opened by SOC are enhanced significantly after the heavier halogen elements introduced, especially in T-SnBr (26.7 meV) and T-SnI (132.5 meV) monolayers, which may provide the feasibility for experimental detection and utilization.
- The nodal-line semimetals and topological insulators can be switched through two sets of the elements (F, Cl and Br, I) decorated.

References: 1. Bzdušek, T., Wu, Q., Rüegg, A. *et al. Nature* **538**, 75–78 (2016). 2. Y. Xu, B. Yan, S. C. Zhang, *et al. PRL*. **111**, 136804 (2013). 3. S. Ghosal and D Jana, *Appl. Phys. Rev.* **9**, 021314 (2022).

2023 Annual Conference of Physics Department

Fudan University

(June 10, 2023 | Shanghai)