Trigonal multivalent polonium monolayers with intrinsic quantum spin Hall effects

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Abstract: The recently successful fabrication of 2D Te monolayer (*i.e.*, tellurene) in experiments has promoted the researches on the group-VI monolayer materials. With first-principles calculations and tight-binding method, we investigate the structures and electronic states of 2D polonium (poloniumene), in which Po is a congener of Te. The poloniumene is found tending to form a three-atomic-layer 1T-MoS_2-like structure (called trigonal poloniumene), namely, the central-layer Po atoms behave metal like, while the two-outer-layer Po atoms are semiconductor like. This unique multivalent behavior of the Po atoms gives rise to the structural stability of the monolayer. The material is found being an intrinsic quantum spin Hall insulator with a large band gap. The nontrivial topology is originated from the $p_{x,y}$–$p_z$band inversion, understood based on a TB model built. The obtained topological state is robust against in-plane biaxial strain and maintains well on a BN substrate. The poloniumene with different congener elements doped are also explored. Our results provide comprehensive understandings of structures, electronic states, and possible applications of 2D polonium-related materials.

Geometry structures and stability

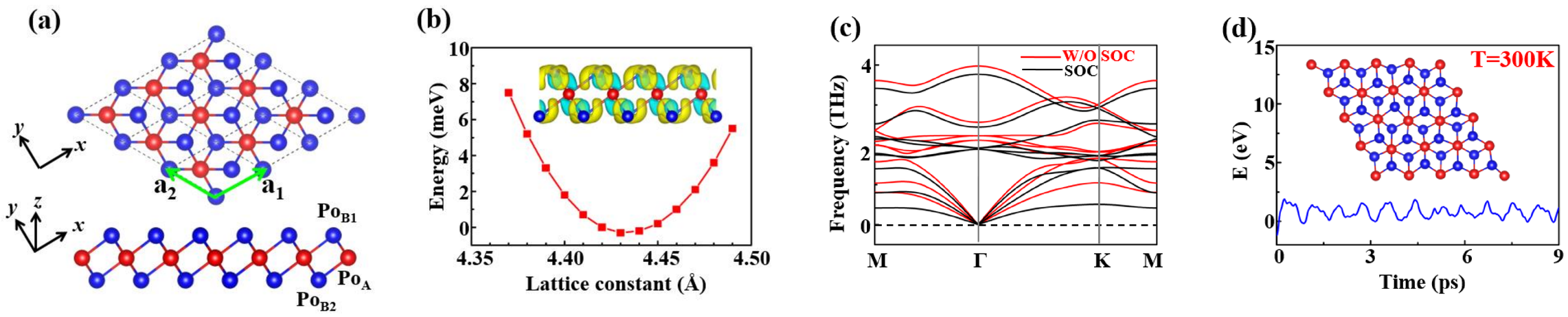


FIG. 1. (a) Top and side views of the trigonal poloniumene. (b) Total energy as a function of the lattice constant,where the total energy (-8.918 eV) is set as zero energy reference. The inset gives the difference of the charge densities. (c) Phonon spectra without and with SOC. (d) Molecular dynamics simulations.

Band structures

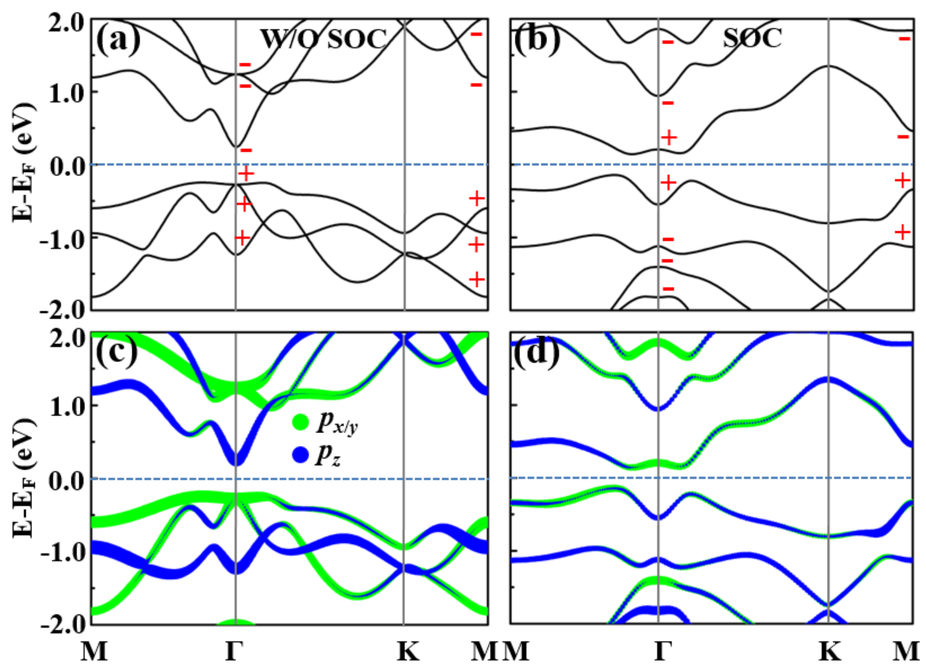


FIG. 2. (a)-(b) Band structures without and with SOC of the trigonal poloniumene, where the red labels + (-) denote even (odd) parity. (c)-(d) Orbital-resolved band structures without and with SOC.

Topological propeties

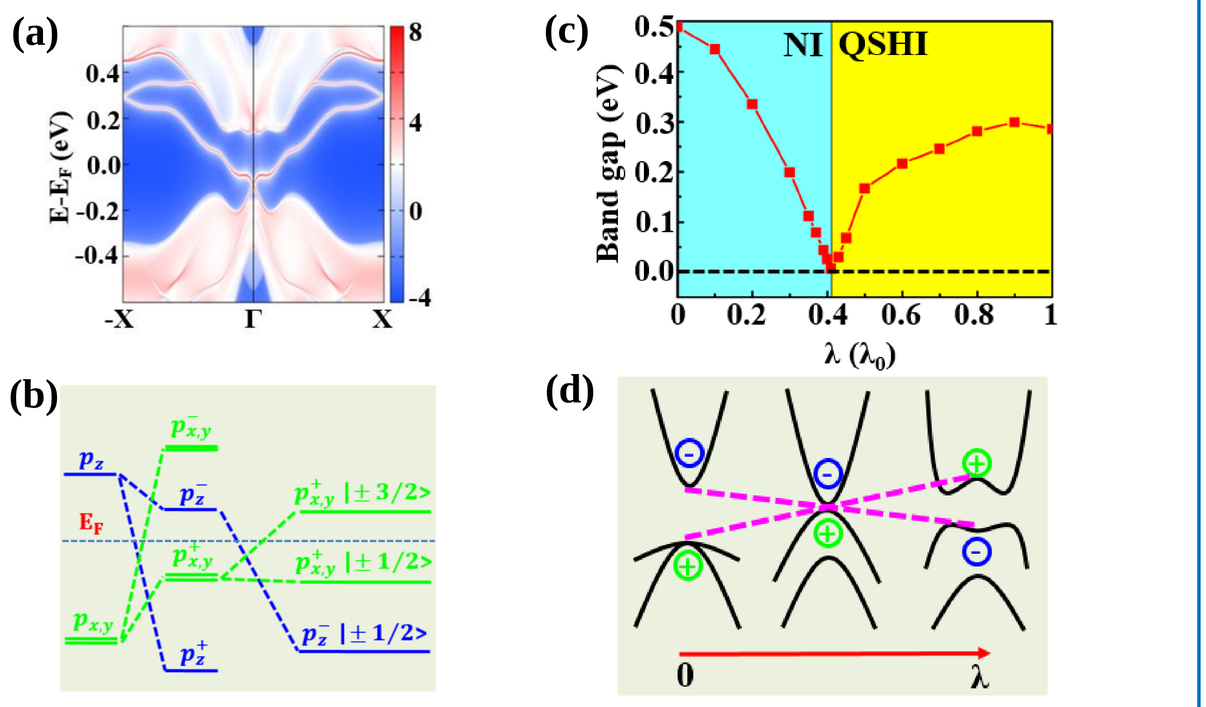


FIG. 3. (a) Helical edge states. (b) Schematic diagram of the energy level evolution for $p_{x,y}$–$p_z$orbitals near Γ point. (c) Indirect band gaps and topological phases versus the SOC. (d) Band inversion mechanism from symmetry analysis and DFT calculations.

Effects of strain, electric field, and substrate

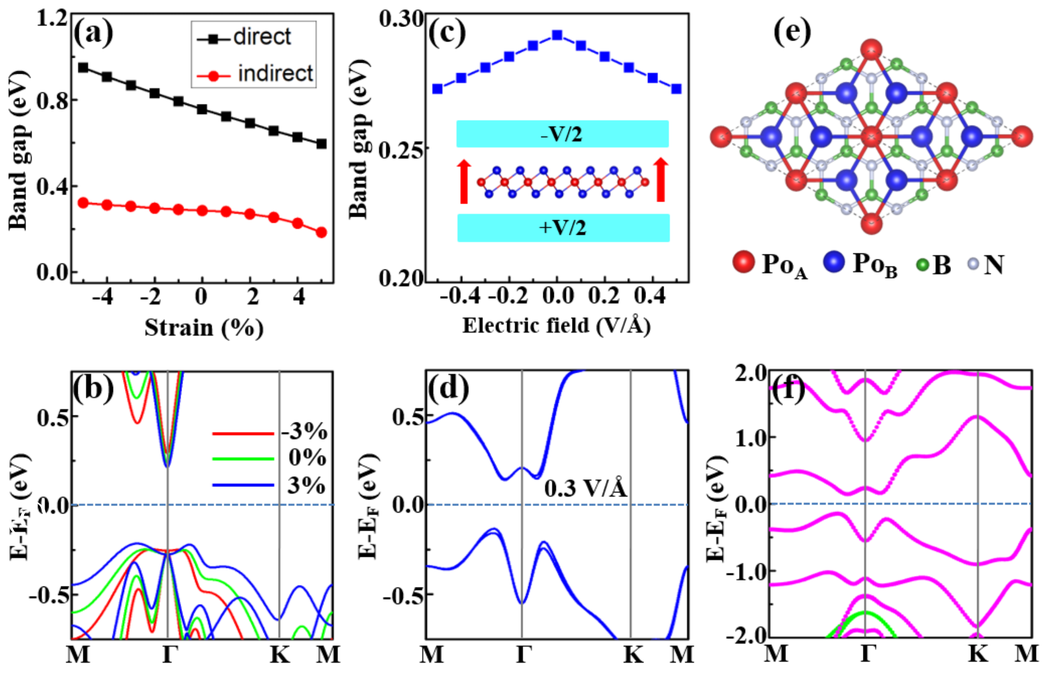


FIG. 4. (a) Direct and indirect band gaps as a function of the in-plane biaxial strain. (b) Band structures without SOC under the different strains. (c) Global band gaps as a function of the external electric field. (d) Band structure with SOC under the electric field of 0.3 V/Å. (e) Top view of the trigonal poloniumene on an h-BN substrate. (f) Band structure of the trigonal poloniumene/h-BN heterostructure with SOC.

Substitutional doping

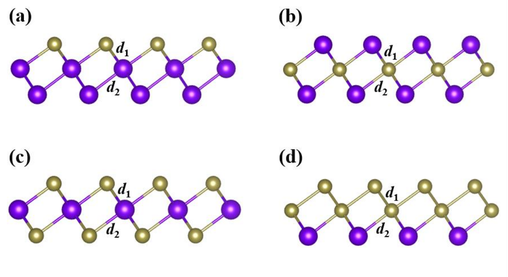
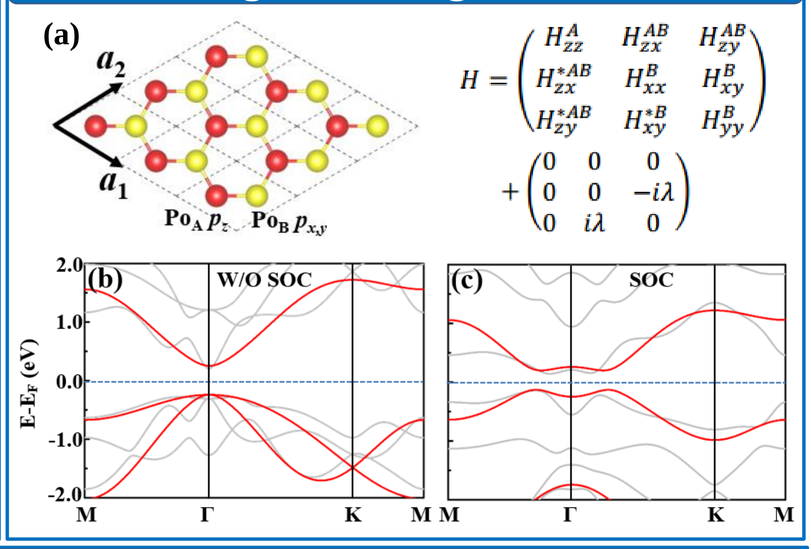


FIG. 5. Geometrical structures for the trigonal poloniumene with four doping patterns of (a) XPoPo, (b) PoXPo, (c) XPoX, and (d) XXPo, in which X=S, Se, Te atoms.

Tight-binding model



Conclusions

I. One trilayer 1T-MoS_2-like structure is proposed for Po films, which is both dynamically and thermally stable.

II. The trigonal poloniumene is an intrinsic topological insulator with a large global band gap, which is identified by the Z_2 invariant, evolution of the Wannier charge center, and the helical edge states.

III. The topological mechanism is ascribed to the $p_{x,y}$–p_z band inversion, explained by a TB model.

IV. Substitutional doping as well as effects of strain, electric field, and substrate on the trigonal poloniumene are explored.

References

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[3] L. Fu *et al.*, Phys. Rev. B **76**, 045302 (2007). [4] J. Zhang *et al.*, Phys. Rev. B **97**, 125430 (2018).