Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplemental Material for "Non-volatile control of topological phase transition in an asymmetric ferroelectric In_2Te_2S monolayer"

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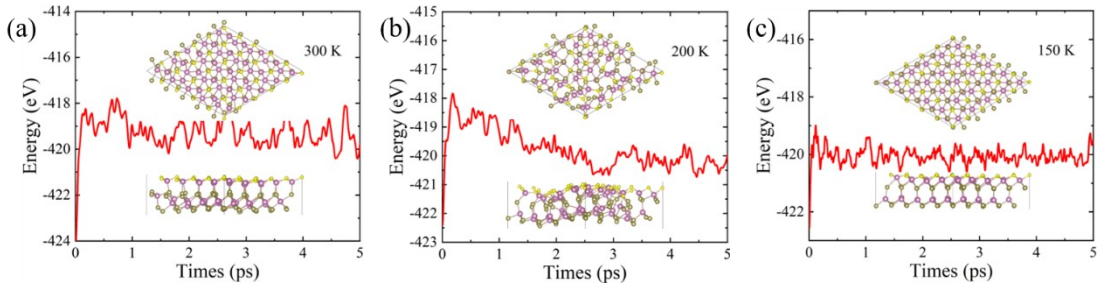

Fig. S1. (a) Snapshots of the atomic configuration at 5 ps and total energy fluctuations for (a) In_2Te_2S monolayer under P (↑) state at 300 K (b) In_2Te_2S monolayer under P (↓) state at 200 K, (c) In_2Te_2S monolayer under P (↓) state at 150 K.

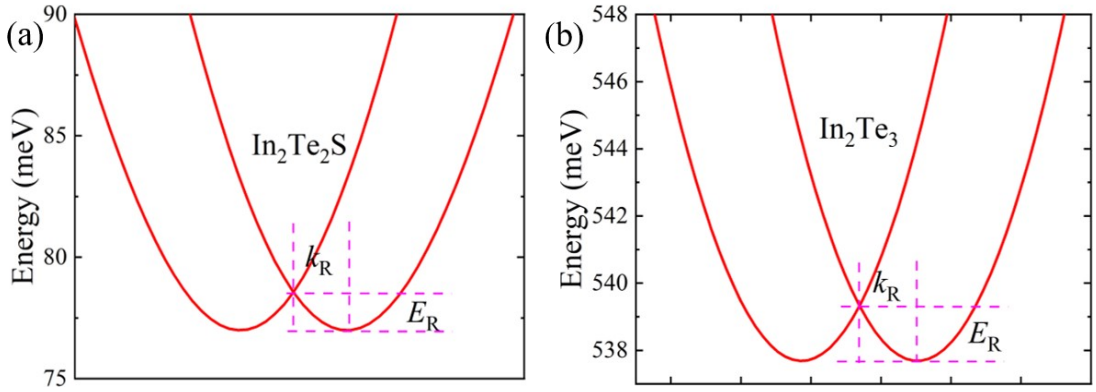

Fig. S2. The Rashba splitting for In_2Te_2S and In_2Te_3 monolayers.

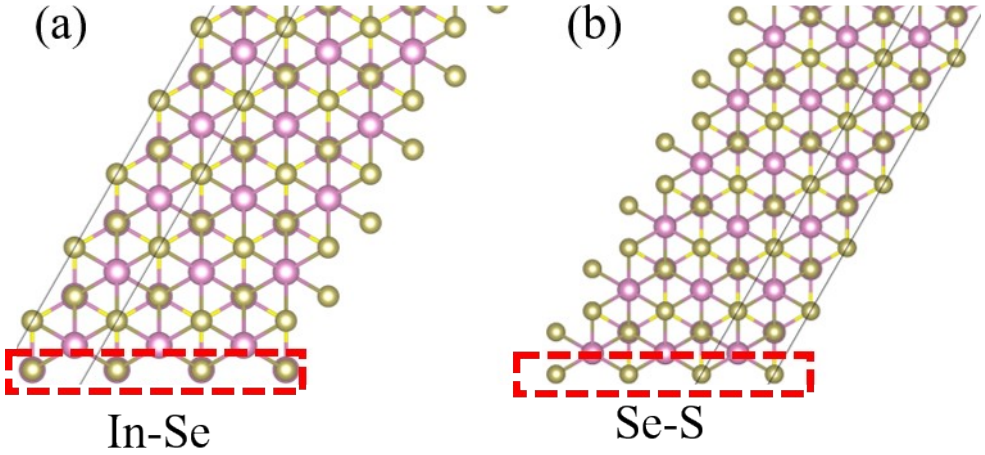

Fig. S3. The crystal structure of different terminal.

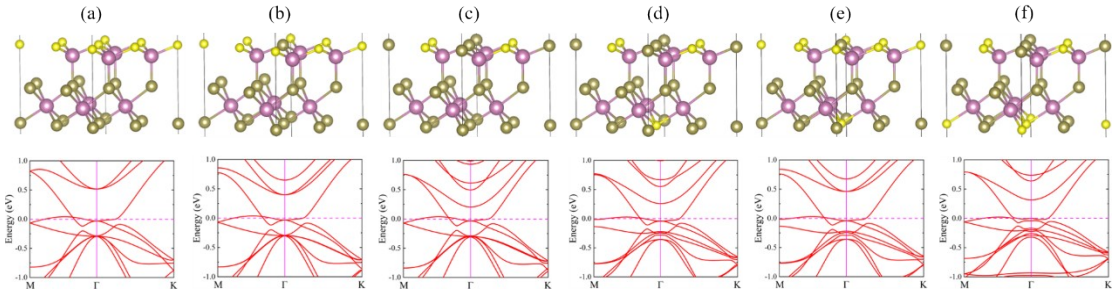

Fig. S4. The calculated band structures for the mixed structure.

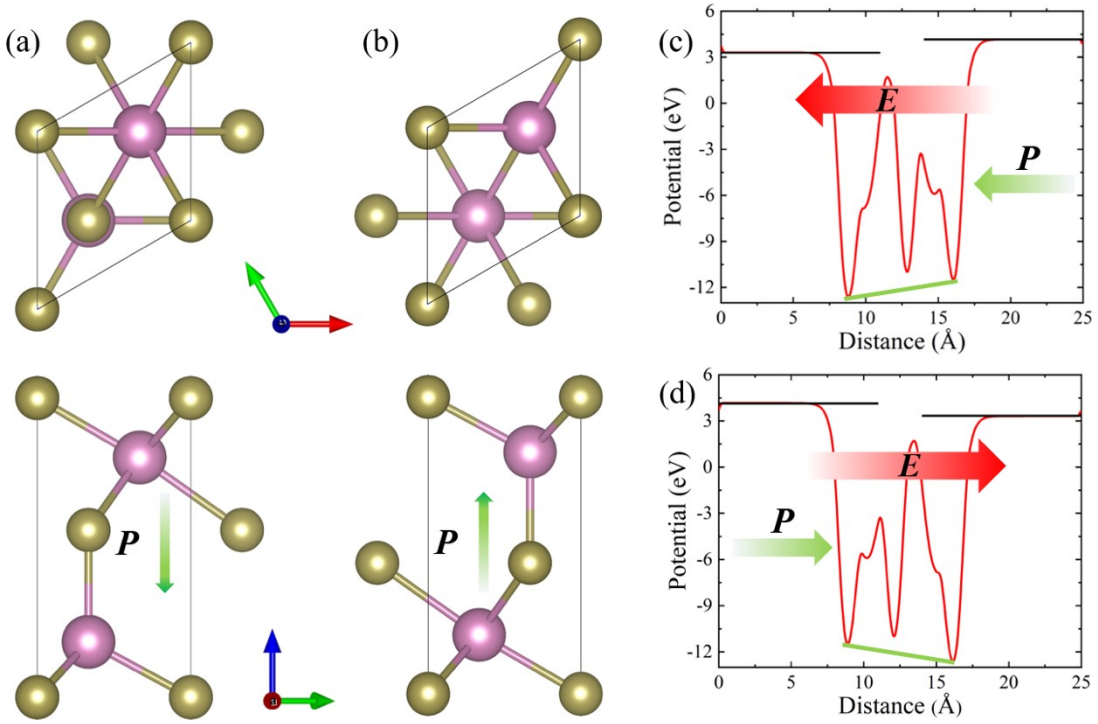

Fig. S5. Crystal structure of In_2Te_3 monolayer under P↓ (a) and P↑ (b). Plane-averaged potential of In_2Te_3 monolayer along its normal, z. (c) P↓. (d) P↑.

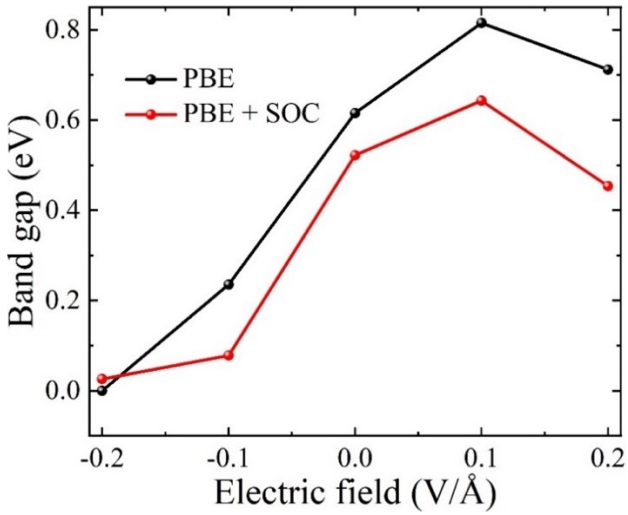

Fig. S6. The calculated band gap as a functional of external electric filed for In_2Te_3 monolayer.

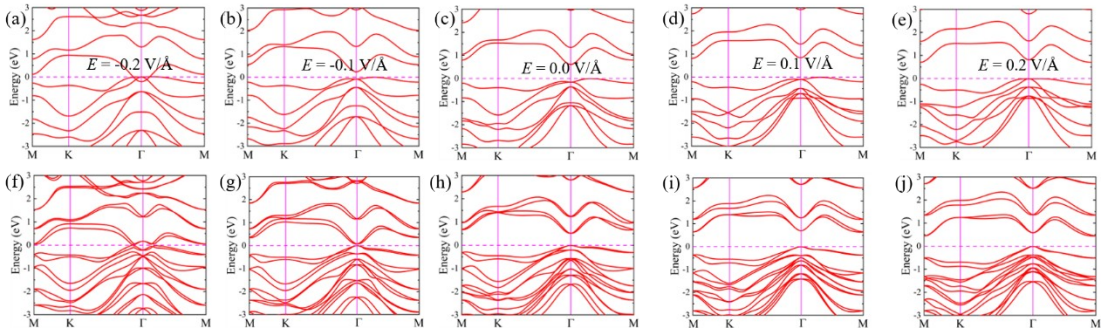

Fig. S7. The calculated band structure as a functional of external electric filed for In_2Te_3 monolayer. (a)-(e) PBE method without SOC. (f)-(j) PBE method with SOC

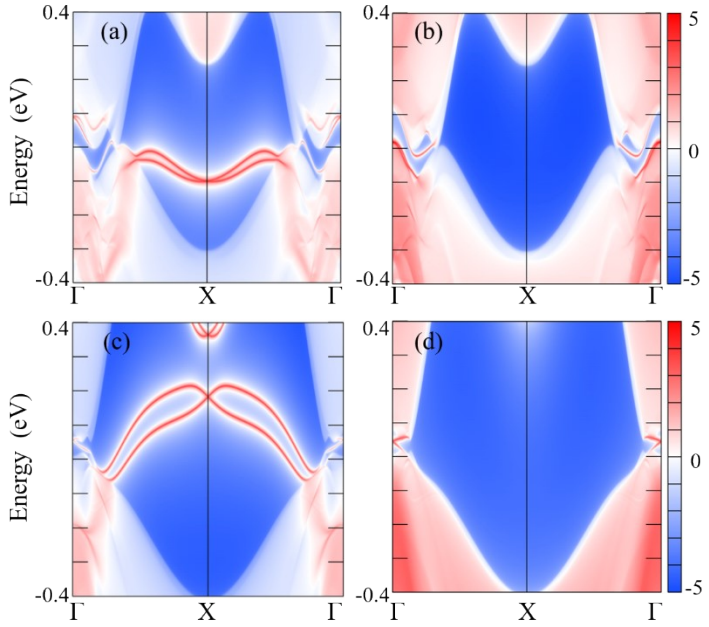

Fig. S8. Topological left (a) and right (b) edge states for In_2Te_2S monolayer under P↑ state at E = -0.1 V/Å. Topological left (c) and right (d) edge states for In_2Te_2S monolayer under P↑ state at E = 0.1 V/Å.

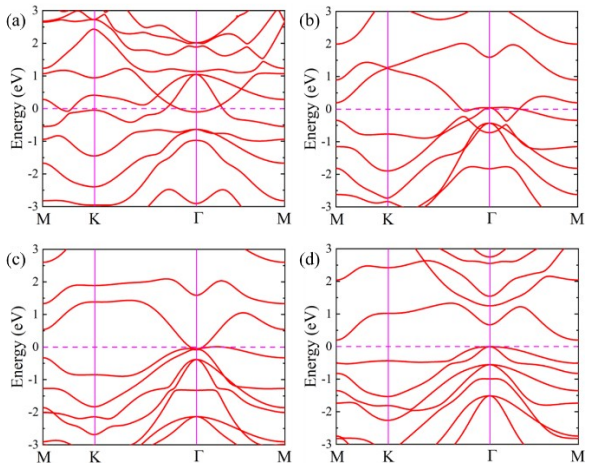

Fig. S9. Band structure of In_2Te_2S monolayer under different electric field. (a) -0.5 V/ Å; (b) -0.1 V/ Å; (c) 0.1 V/ Å; (d) 0.5 V/ Å.

Table SI. The calculated lattice parameters for In_2Te_2S and In_2Te_3 monolayers. The 1, 2, 3, 4, and 5 represent the S (Te), In, Te, In, and Te atoms.

	a (Å)	*h* (Å)	1-2	2-3	3-4	4-5
In_2Te_2S-up	4.227	7.187	2.682	3.068	2.750	2.847
In_2Te_2S-down	4.224	7.182	2.626	2.795	3.056	2.901
In_2Te_3-up	4.406	7.403	2.938	3.112	2.767	2.890
In_2Te_3-down	4.406	7.403	2.890	2.767	3.112	2.938

Table SII. The calculated charge for different atom with Bader method.

	Te	In	Te	In	S
In_2Te_2S-up	6.405	2.288	6.486	2.071	6.750
In_2Te_2S-down	6.443	2.371	6.477	2.000	6.707
In_2Te_3-up	6.413	2.368	6.480	2.284	6.453
In_2Te_3-down	6.453	2.284	6.480	2.368	6.413