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

Prediction of Topological Crystalline Insulator and Topological Phase Transitions in Two-dimensional PbTe Films

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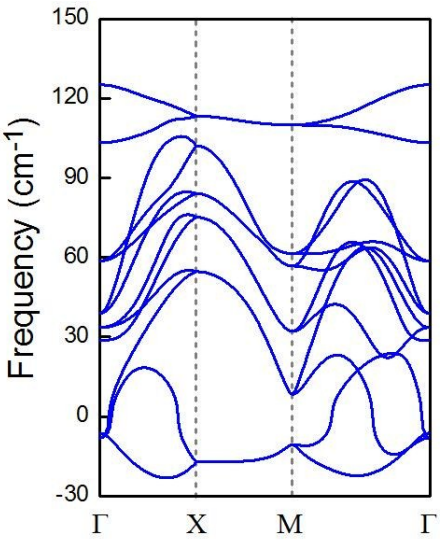

Fig. S1 Calculated phonon band dispersions of PbTe monolayer.

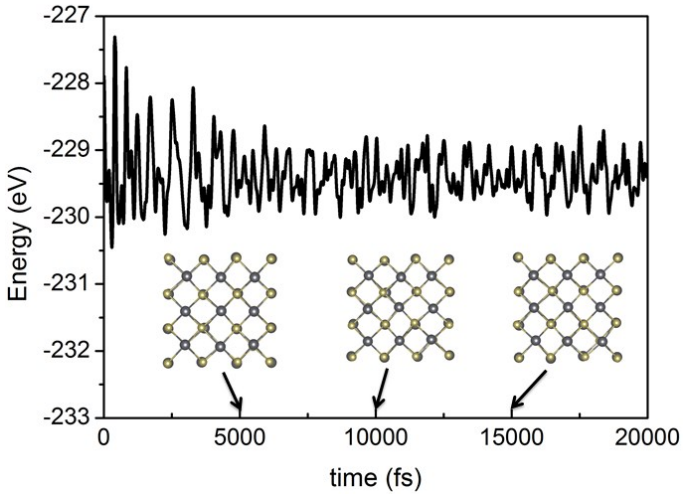

Fig. S2 Snapshots of atomic configurations of PbTe bilayer at the end of MD simulation at 5, 10 and 15 ps, respectively. The total potential energy fluctuation during MD simulations is calculated at 300K.

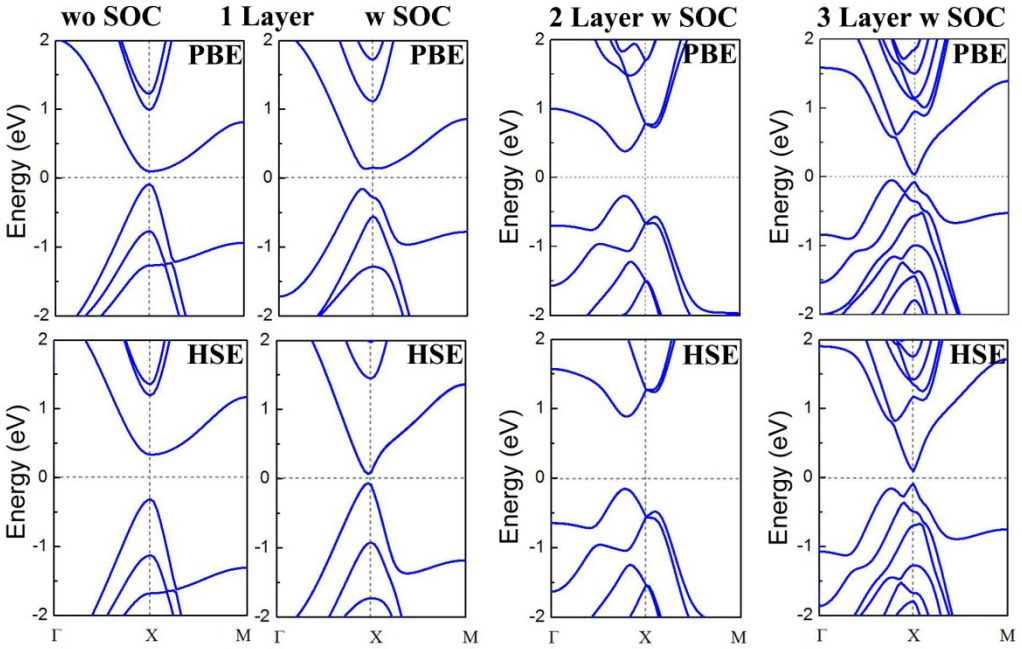

Fig. S3 Calculated band structures with HSE06 for monolayer, bilayer, and trilayer, respectively.

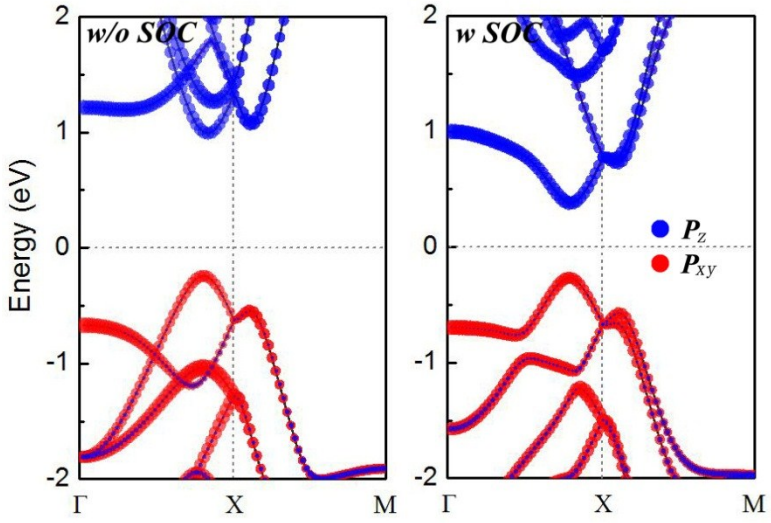

Fig. S4 Orbital-resolved band structures for bilayer, with and without considering SOC respectively, weighted with the Te-$p_{x,y}$ and Pb-p_z characteristics.

Fig. S5 The corresponding structural information on POSCAR in our calculations:

(a) POSCAR of monolayer

1.00000000000000

4.4889228056552579 0.0000000000000000 0.0000000000000000

0.0000000000000000 4.4889228056515705 0.0000000000000000

0.0000000000000000 0.0000000000000000 23.2953441136542807

Te Pb

1 1

Direct

0.5000000000000000 0.5000000000000000 0.5000000000000000

0.0000000000000000 0.0000000000000000 0.5000000000000000

(b) POSCAR of bilayer

1.00000000000000

4.4764540341984835 0.0000000000000000 0.0000000000000000

0.0000000000000000 4.4764540341984835 0.0000000000000000

0.0000000000000000 0.0000000000000000 27.3528808412564679

Te Pb

2 2

Direct

0.0000000000000000 0.0000000000000000 0.5546725080417048

0.5000000000000000 0.5000000000000000 0.4497122475074988

0.0000000000000000 0.0000000000000000 0.4497122475074988

0.5000000000000000 0.5000000000000000 0.5546725080417048

(c) POSCAR of trilayer

1.00000000000000

4.3924071424175182 0.0000000000000000 0.0000000000000000

0.0000000000000000 4.3924071424175182 0.0000000000000000

0.0000000000000000 0.0000000000000000 28.4096677127749189

Te Pb

3 3

Direct

0.0000000000000000 0.0000000000000000 0.4999038111126973

0.5000000000000000 0.5000000000000000 0.3949435505784914

0.5000000000000000 0.5000000000000000 0.6048640716469104

0.0000000000000000 0.0000000000000000 0.3949435505784914

0.0000000000000000 0.0000000000000000 0.6048640716469104

0.5000000000000000 0.5000000000000000 0.4999038111126973

(d) POSCAR of tetralayer

1.00000000000000

4.3765572323085973 0.0000000000000000 0.0000000000000000

0.0000000000000000 4.3765572323085973 0.0000000000000000

0.0000000000000000 0.0000000000000000 28.6158142476331783

Te Pb

4 4

Direct

0.0000000000000000 0.0000000000000000 0.4450198697328935

0.0000000000000000 0.0000000000000000 0.6549403908013124

0.5000000000000000 0.5000000000000000 0.3400596091986876

0.5000000000000000 0.5000000000000000 0.5499801302671065

0.0000000000000000 0.0000000000000000 0.3400596091986876

0.0000000000000000 0.0000000000000000 0.5499801302671065

0.5000000000000000 0.5000000000000000 0.4450198697328935

0.5000000000000000 0.5000000000000000 0.6549403908013124