Supporting Information for

Large gap two Dimensional Topological Insulator from bilayer triangular lattice TlM(M = N, P, As, Sb)

P. Zhou,[1] Lin Xue,[2] and L. Z. Sun[2,*]

[1]*Key Laboratory of Low-dimensional Materials and Application Technology, School of Material Sciences and Engineering, Xiangtan University, Xiangtan 411105, China*
[2]*Hunan Provincial Key laboratory of Thin Film Materials and Devices, School of Material Sciences and Engineering, Xiangtan University, Xiangtan 411105, China*

(Dated: March 17, 2017)

PACS numbers: 71.20.-b, 71.70.Ej, 73.20.At

I. SNAPSHOTS OF ATOMIC CONFIGURATION AND ENERGY CHANGES UNDER 500K AND 800K MD SIMULATIONS.

We plot the snapshots of atomic configuration after NVT simulation and energy changes under 500K and 800K during the process of MD simulations. They clearly indicate that the bilayer hexagonal lattice own great stability with temperature fluctuation.

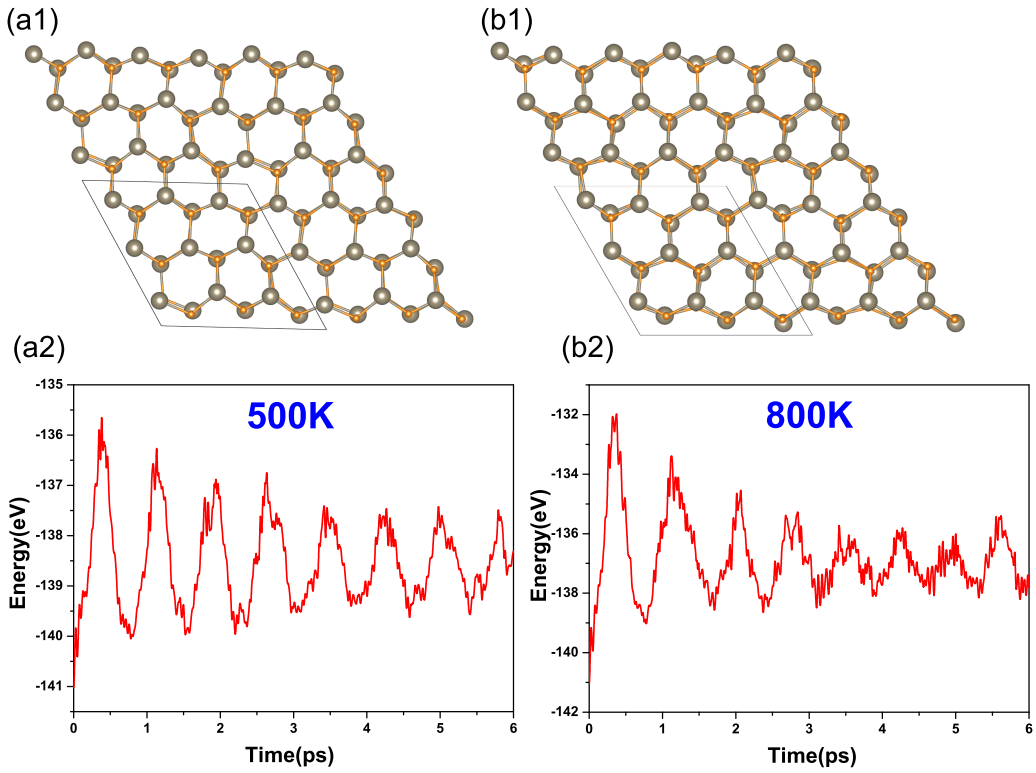

Figure S1: (color online) The snapshots of atomic configurations of TlM 2D crystal at the end of MD simulations at (a1) 500 K and (b1) 800 K. (a2) and (b2) are the energy changes with times under previous two MD's temperature, respectively.

II. ENERGY BAND WITH PBE AND HSE06 EXCHANGE CORRELATION FUNCTION WITHOUT SOC

The energy band with PBE and HSE06 exchange correlation functional without SOC for all four structure we considered are ploted in following figure. Except shifting the extreme point along Γ-K high symmetry line down to

Γ degenerate point around Fermi level for TlN, HSE06 function's energy band share similar characters with PBE results.

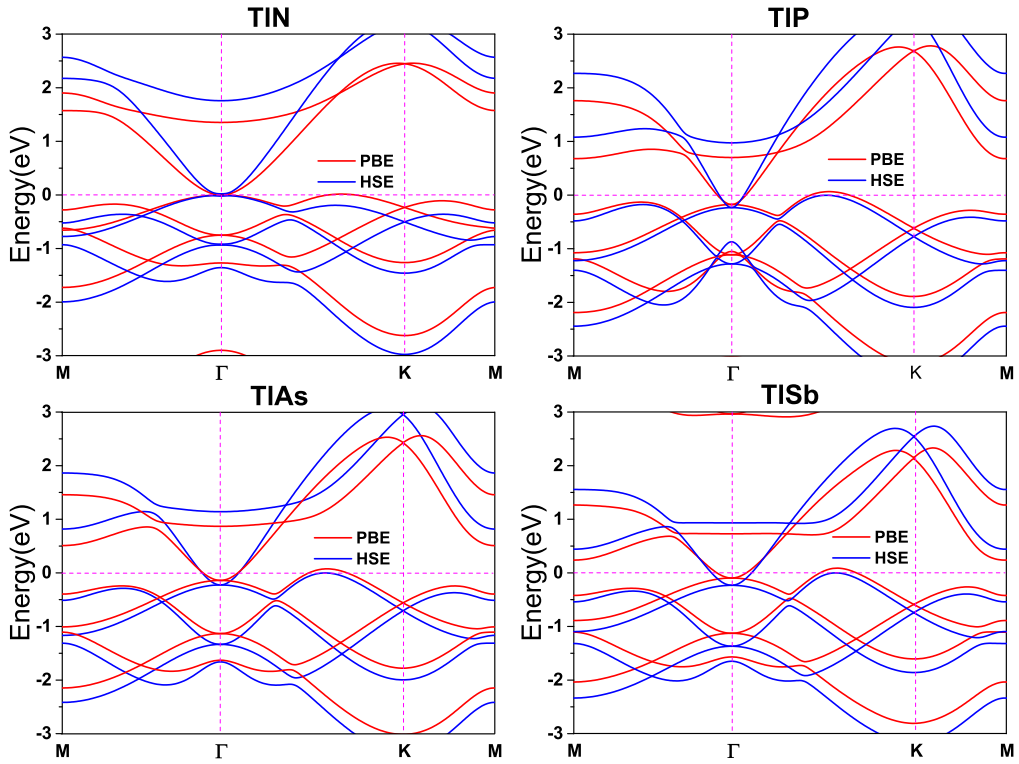

Figure S2: (color online) Energy band with PBE and HSE06 exchange correlation function without SOC for all bilayer TlM.

III. THE P_z PROJECTED ENERGY BAND WITH INCREASING THICKNESS OF BILAYER TLN

The p_z projected energy band with increasing thickness of bilayer TlN. The label represent the increased thickness compared with bilayer materials' inherent thickness h, which are listed in Table I of main text.

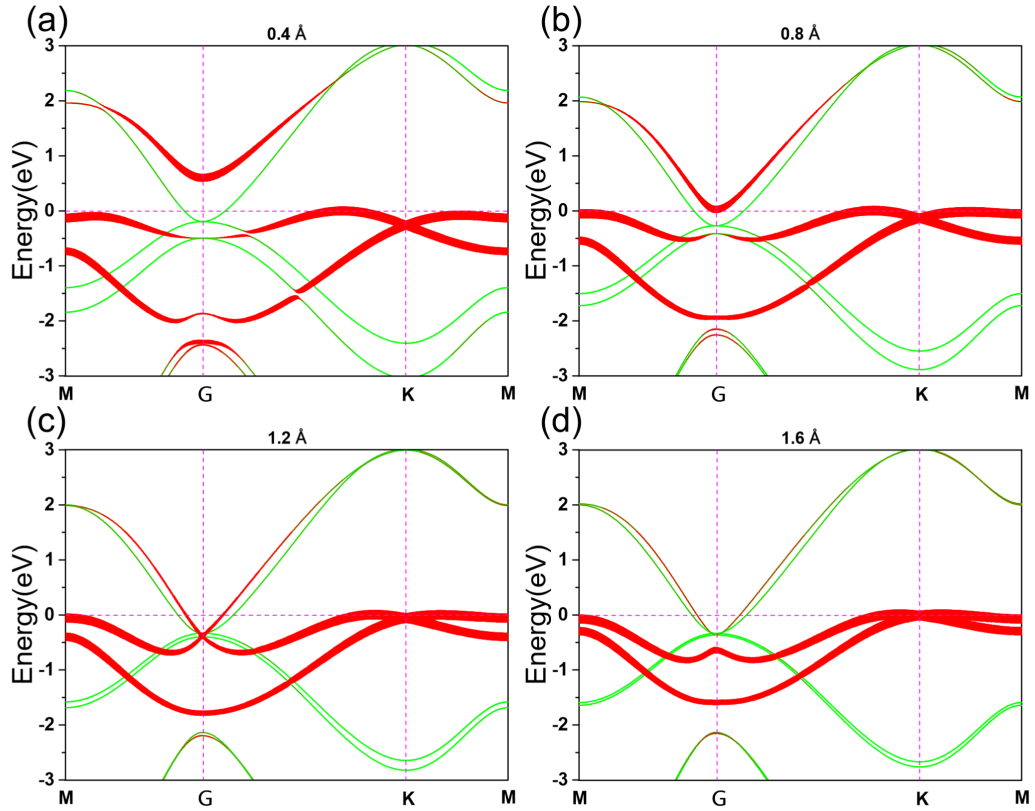

Figure S3: (color online) The p_z projected energy band with increasing thickness of bilayer TlN.

IV. ENERGY BAND EVOLUTION WITH DIFFERENT STRAIN

Energy band evolution with different strain. Negative value mean compression stress and positive value represent tensile stress. The green arrow represent the move of extreme point along Γ-K high symmetry line.

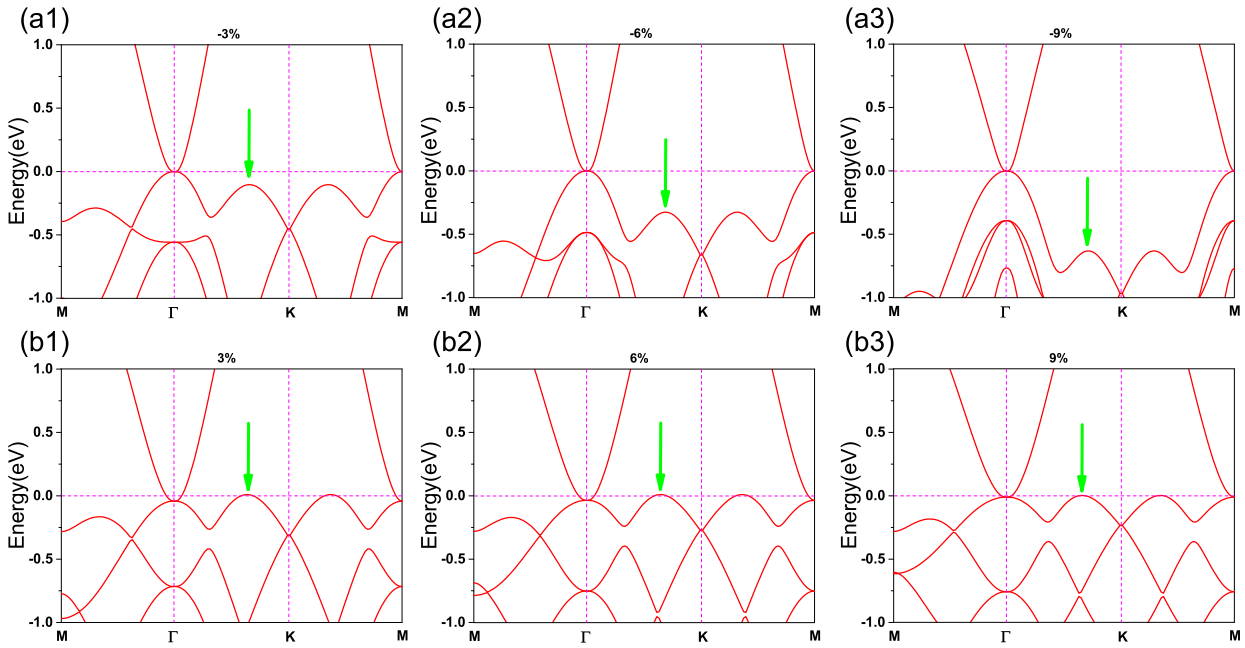

Figure S4: (color online) Energy band evolution with different strain. Negative value mean compression stress and positive value represent tensile stress.

V. ENERGY BAND STRUCTURE FOR THREE LAYER AND FOUR LAYER TLN

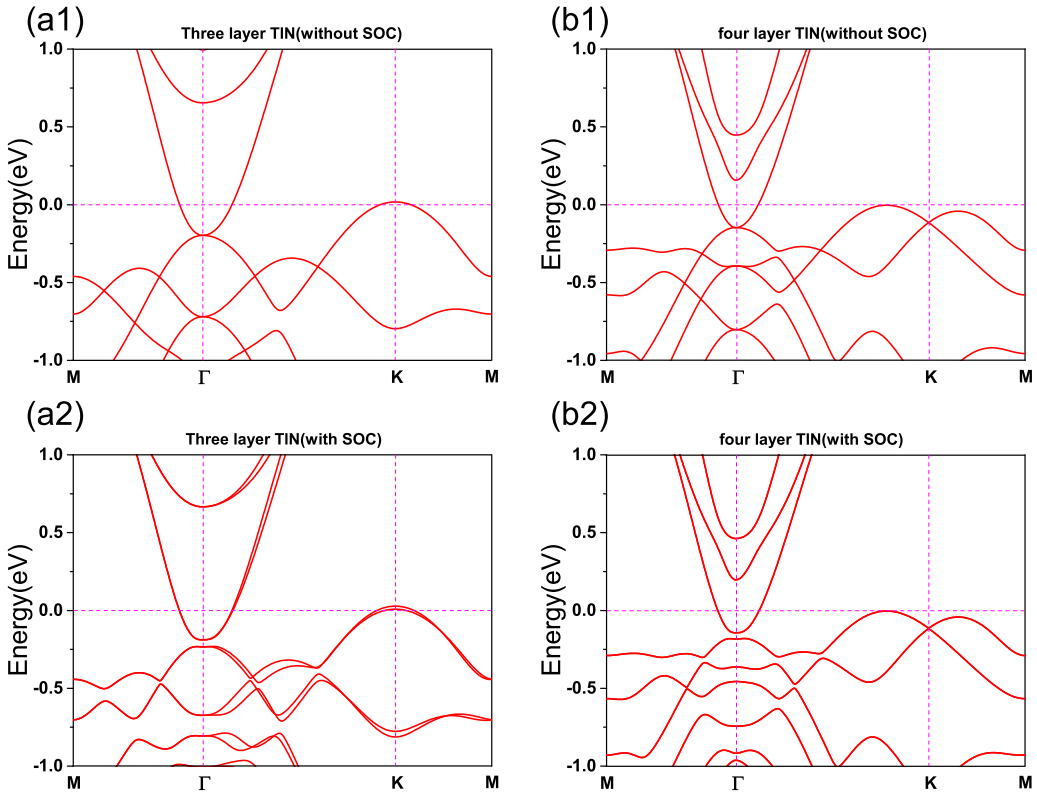

Figure S5: (color online) Energy band structure for three layer and four layer TlN without SOC and with SOC.

VI. ENERGY BAND STRUCTURE OF SURFACE HYDROGENATION TL OR N FOR BILAYER TLN

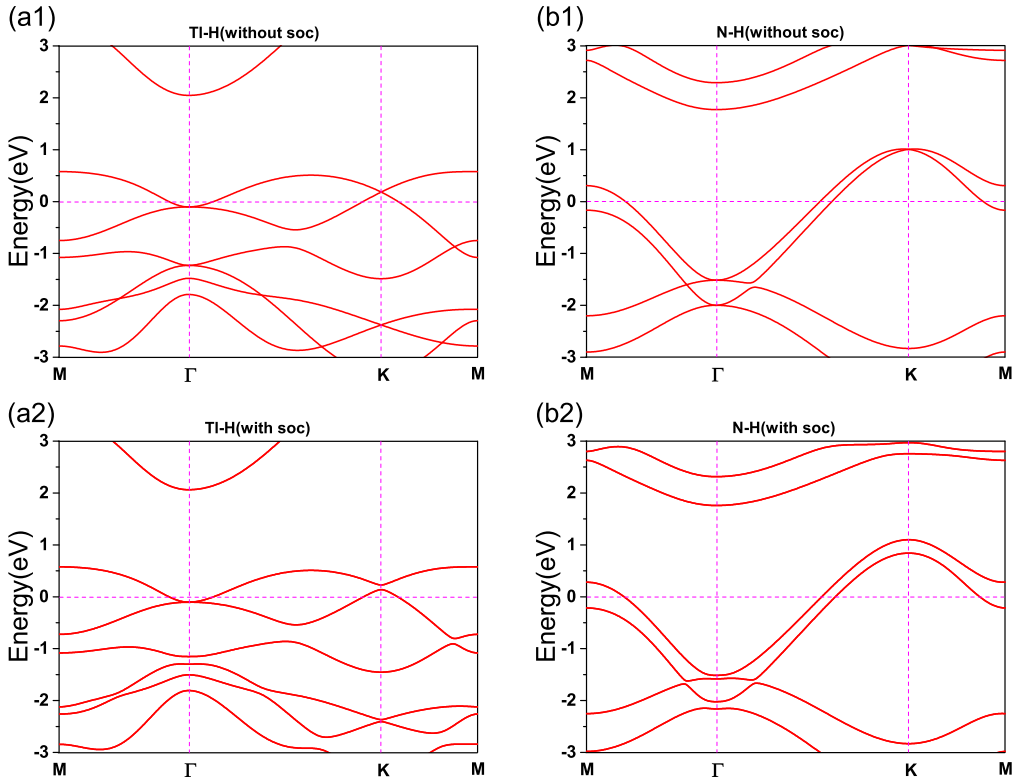

Figure S6: (color online) Energy band structure of surface hydrogenation Tl or N for bilayer TlN without SOC and with SOC.

* Electronic address: lzsun@xtu.edu.cn