Electronic Supplementary Material (ESI) for Nanoscale.

Electronic Supplementary Information

Prediction of topological nontrivial semimetals and pressure-induced Lifshitz transition in 1T'-MoS_2 layered bulk polytypes

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In the stacking process of 1T' monolayer, there are translational and rotational degrees of freedom between the two layers. Rotate the upper layer of 2M-MoS_2 180 degrees around the b axis and then translate it can reproduce the bottom layer. For the β-MoS_2, rotate 180 degrees of the upper layer around a-axis followed by translation can reproduce the second layer. The following table list the four configurations labeled by 2M, 1T', β, and T_d-MoS_2.

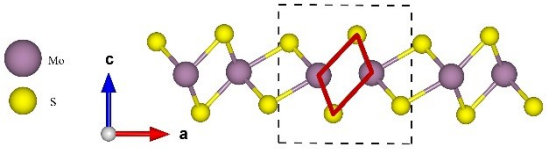
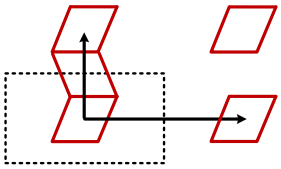
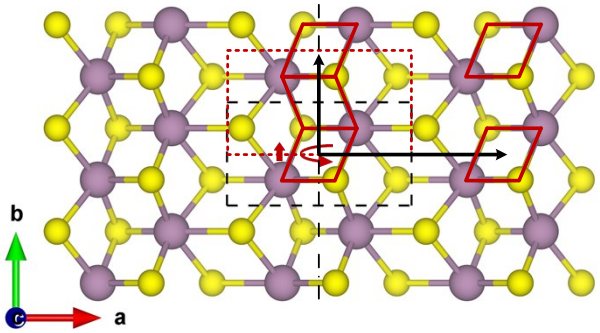
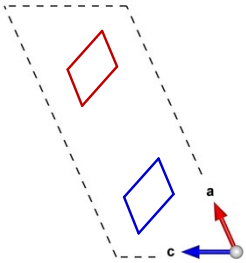
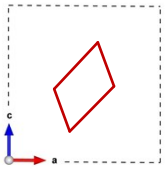
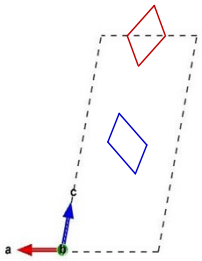
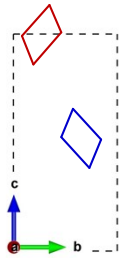
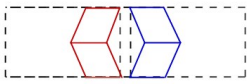
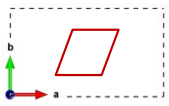
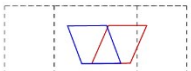
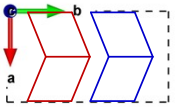
Side view				
Top view				
Rotation Translation	{0|0}	1T'-MoS_2 Monolayer		
	2M-C2/m	1T'-$P2_1/m$	β-$P2_1/m$	T_d-$Pnm2_1$
Side view				
Top view				
Rotation Translation {R|t_a t_b t_c}	{R_b: π| 0.5 0 0}	{0|0}	{R_a: π| 0 0 0.5}	{R_b: π| 0 0.5 0.5}
Symmetry	spoil screw symmetry of monolayer	maintain screw symmetry of monolayer		break inversion

Figure S1. 1T'-monolayer of MoS_2 and layered bulk structures through lateral rotation and

translation between layers. Red and green represent the top and bottom layer of the bilayer, respectively.

Table S1. Relaxed four bulk polytypes of MoS_2 at ambient pressure without the inclusion of SOC.

Phase	Space Group	Lattice Parameter (Å)	Atom	Wyckoff Position	Atomic Coordinates		
					X	Y	Z
2M	***C2/m***	**a= 12.9285**	**Mo**	**4i**	**-0.2429**	**0**	**0.2942**
		b= 3.1759	**S1**	**4i**	**-0.8613**	**0**	**0.1809**
		c= 5.7199	**S2**	**4i**	**-0.6045**	**0**	**0.2882**
		α=γ=90° β=66.09°					
1T′	***$P2_1/m$***	**a= 5.7250**	**Mo**	**2e**	**0.6996**	**0.75**	**0.5103**
		b=3.1847	**S1**	**2e**	**0.4108**	**0.75**	**0.2145**
		c=5.9526	**S2**	**2e**	**0.9205**	**0.25**	**0.2766**
		α=γ=90° β=90.46°					
β	***$P2_1/m$***	**a= 5.7142**	**Mo1**	**2e**	**0.7022**	**0.25**	**0.5052**
		b=3.1730	**Mo2**	**2e**	**0.3013**	**0.25**	**0.0058**
		c=12.3213	**S1**	**2e**	**0.3569**	**0.25**	**0.3589**
		α=γ=90°	**S2**	**2e**	**0.1220**	**0.25**	**0.6104**
		β=100.80°	**S3**	**2e**	**0.5243**	**0.25**	**0.8591**
			S4	**2e**	**0.9655**	**0.25**	**0.1105**
T_d	***$Pmn2_1$***	**a=3.1752**	**Mo1**	**2a**	**0**	**0.1034**	**0**
		b=5.7178	**Mo2**	**2a**	**0**	**0.4978**	**0.5132**
		c=11.9241	**S1**	**2a**	**0**	**0.3822**	**0.1506**
		α=β=γ=90°	**S2**	**2a**	**0**	**0.1182**	**0.6171**
			S3	**2a**	**0**	**0.7789**	**0.3624**
			S4	**2a**	**0**	**0.7239**	**0.8961**

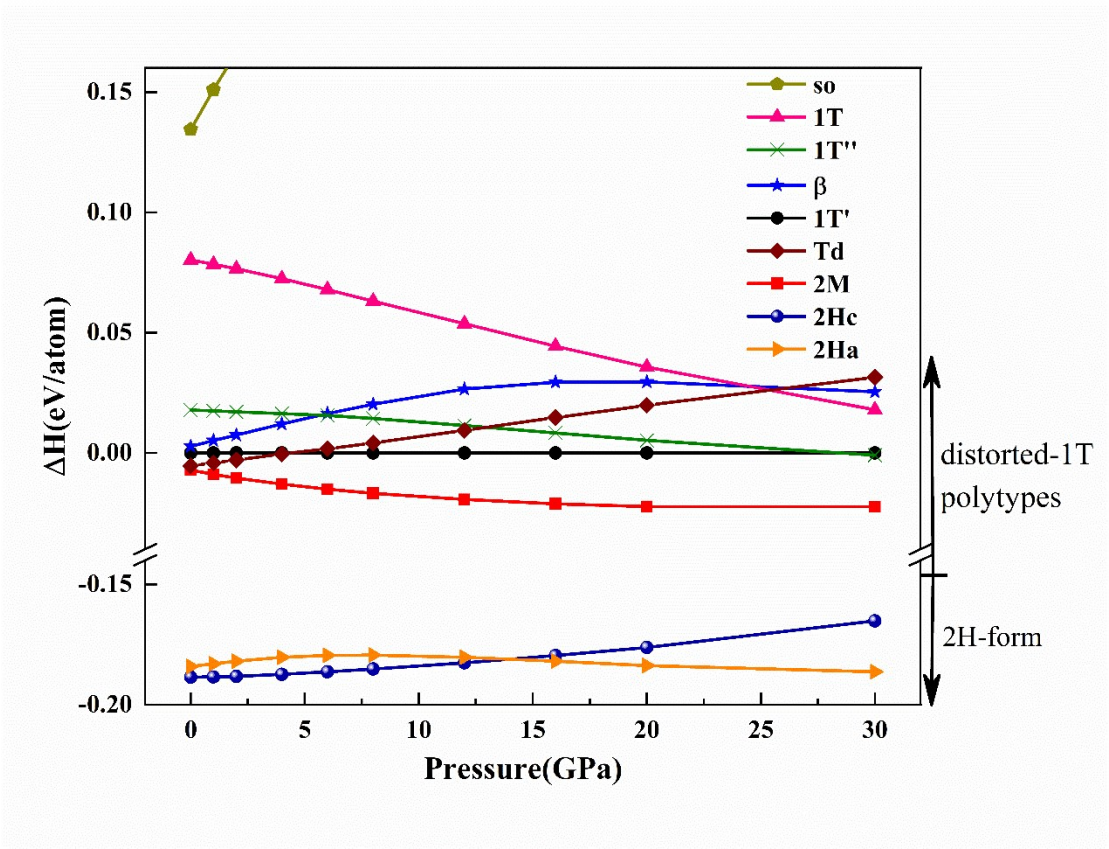


Figure S2. The enthalpy curves (relative to bulk 1T'-$P2_1/m$) for various bulk structures in the pressure range of 0-30GPa.

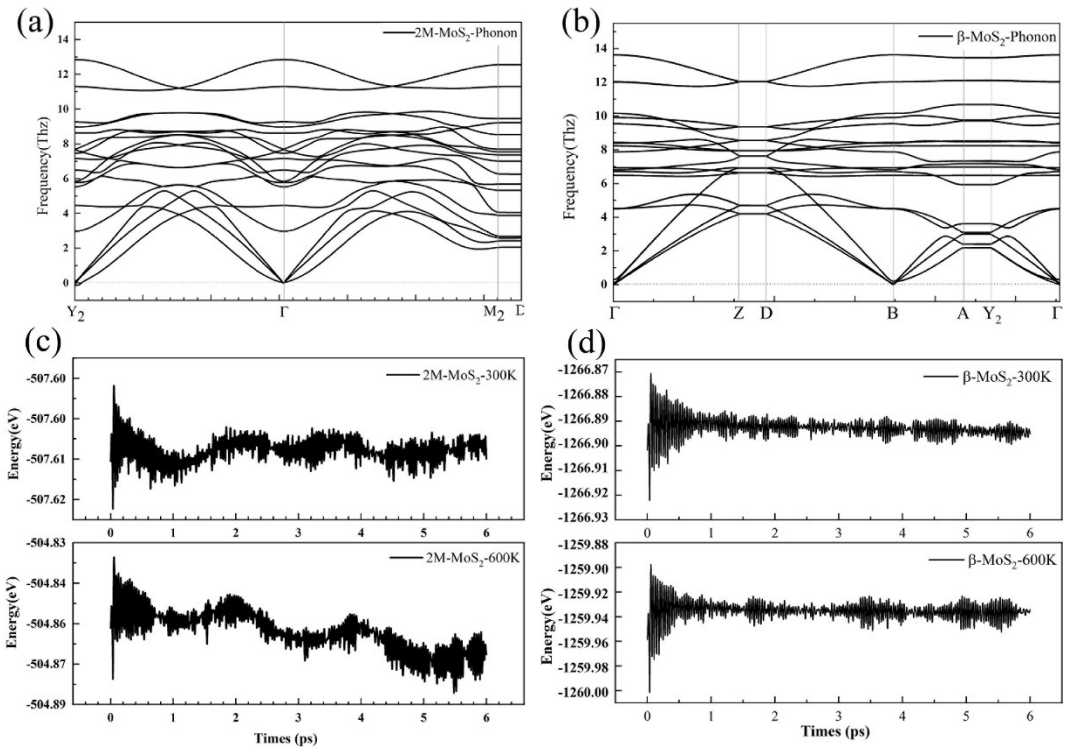


Figure S3. Calculated phonon dispersion of (a) 2M-MoS_2 and (b) β-MoS_2. AIMD simulation for (c) 2M-MoS_2 and (d) β-MoS_2 at 300 and 600K.

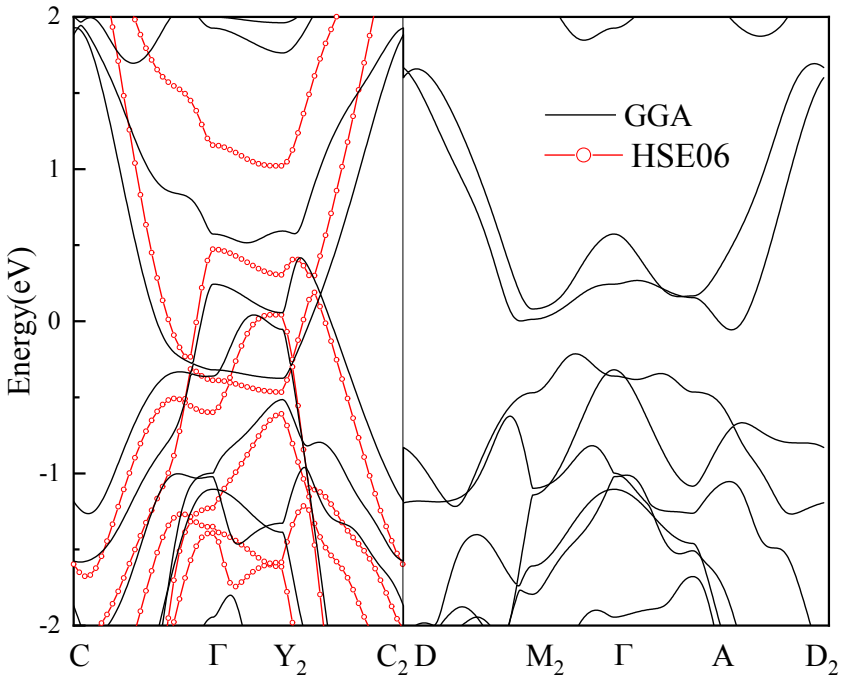


Figure S4. The band structures of 2M-MoS_2 calculated within GGA (black lines) and hybrid functional HSE06 (red circled lines).

The electronic fillings of bulk 1T'-MoS2 with a nonsymmorphic space group of 11 fulfill the filling constraints for the gapless system. The gapless point is located at the high symmetry path of Γ-Z as shown in Fig. S5(a), which is topological protected by the screw symmetry of Sy. In fact, the shape of the band structure (marked in blue) can be seen as a distorted hourglass, thus it is analogous to the spinless hourglass nodal-line semimetals. Similar to the case in 2M-MoS2, the coexistence of open and closed type nodal lines is found in the bulk 1T'-MoS2(see Fig.S5(b)). A drumhead-like surface state surrounded by the closed nodal loop near B point appears on the (100) surface of 1T'-MoS2 in Fig.S5(c).

In contrast to the 2M- and 1T'-MoS2, the β-MoS2 possesses two pairs of closed nodal loop shown in Fig. S5(d). Interestedly, double drumhead-like surface sates appear inside the overlapped region of NL1 on the (001) surface of β-MoS2 in Fig. S5(e). The isoenergy surfaces with E=0.21eV and 0.46eV are shown in Fig.S5(f) and S5(g). It should be noted that this drumhead-like surface sates are nearly flat and cover a larger part of BZ, partially fulfilling the aforementioned characteristics of good candidates.

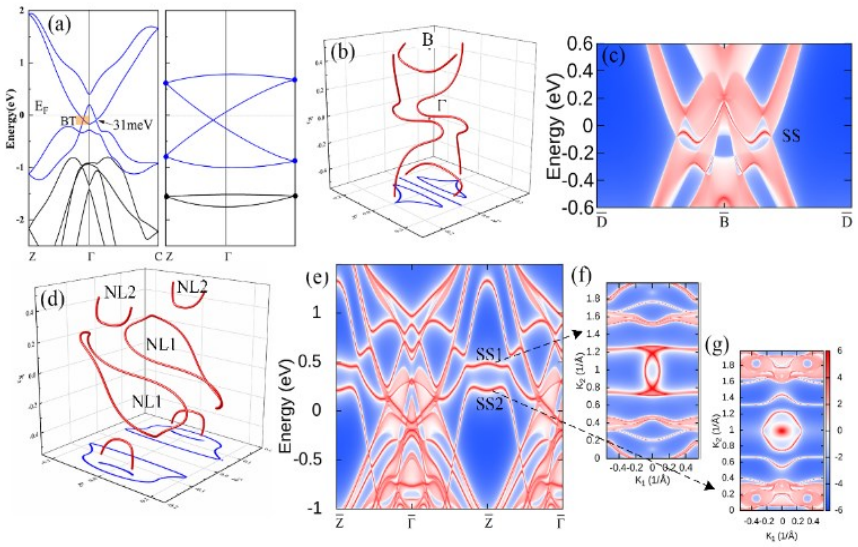


Figure S5. (a) calculated energy band for bulk 1T'-MoS2 and a typical hourglass energy band in nodal line semimetal. (b) calculated band touching points (nodal line) in 3D k space of bulk 1T'-MoS2. (c) calculated surface state on the (100) surface of bulk 1T'-MoS2. (d) nodal line in β-MoS2. (e) surface state and (f) (g) isoenergy surface on the (001) surface of β-MoS2 with E=0.21eV and 0.46eV.

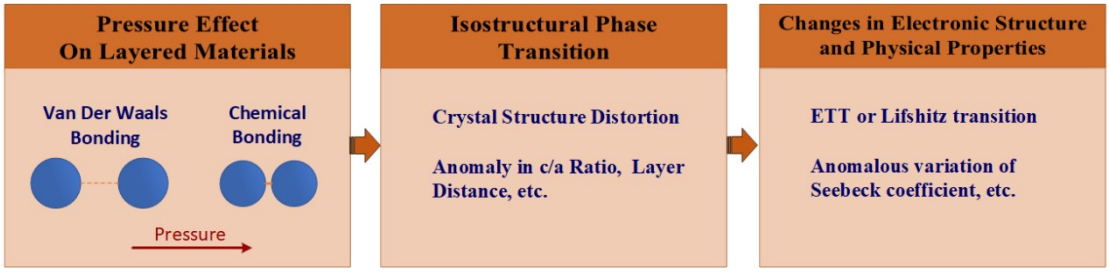


Figure S6. The pressure effect on layered materials and the inherent correlation between structure distortion and electronic topological transition (ETT) or Lifshitz transition.