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

Electronic Supplementary Information

Square transition-metal carbides MC_6 (M = Mo, W) as stable two-dimensional Dirac cone materials

Peng-Fei Liu,[a,b] Yang Wu,[a,b] Tao Bo,[a,b] Ling Hou,[a,b] Juping Xu,[a,b] Hui-jie Zhang,[a,b] and Bao-Tian Wang,[*a,b]

[a]*Institute of High Energy Physics, Chinese Academy of Sciences (CAS), Beijing 100049, China.*

[b]*Dongguan Neutron Science Center, Dongguan 523803, China.*

[*] Corresponding author. Tel.: +86-0411-84986080. E-mail: wangbt@ihep.ac.cn

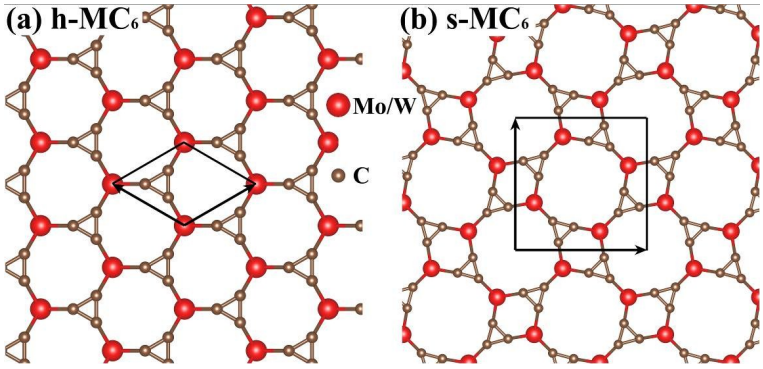

Figure S1. The geometric structures of (a) h-MC_6 and (b) s-MC_6 monolayers.

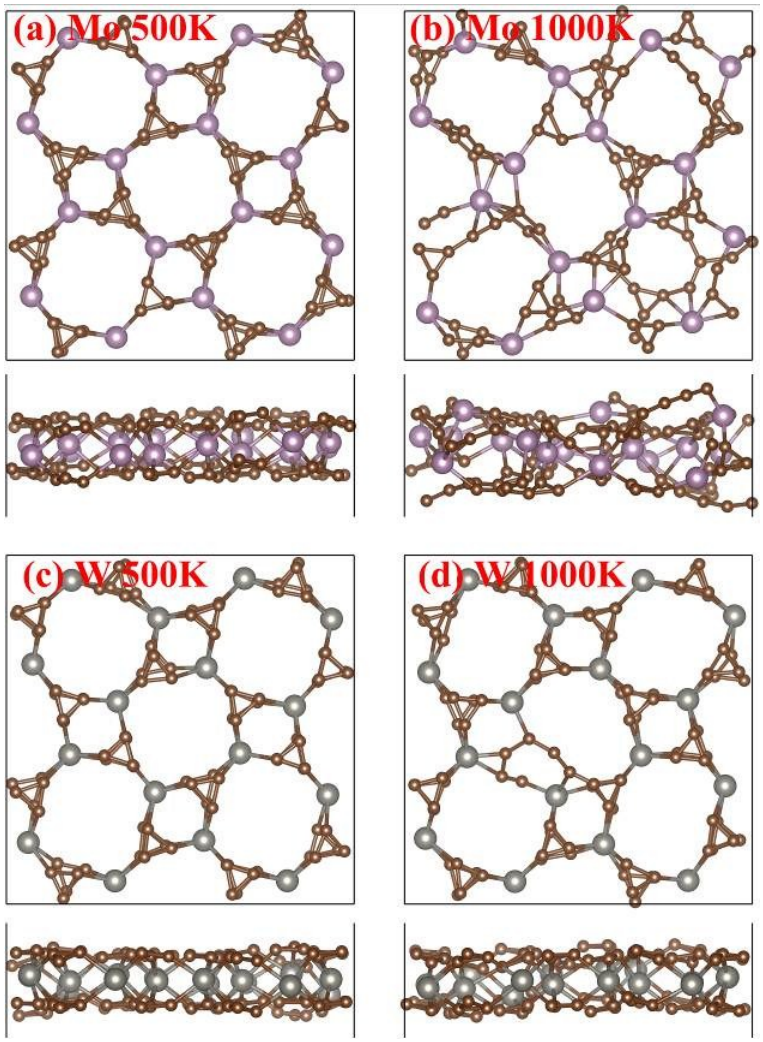

Figure S2. The top and side views of monolayers after the *ab-initio* molecular dynamics simulation. (a) 500 K and (b) 1000 K for s-MoC_6 monolayer. (c) 500 K and (d) 1000 K for s-WC_6 monolayer.

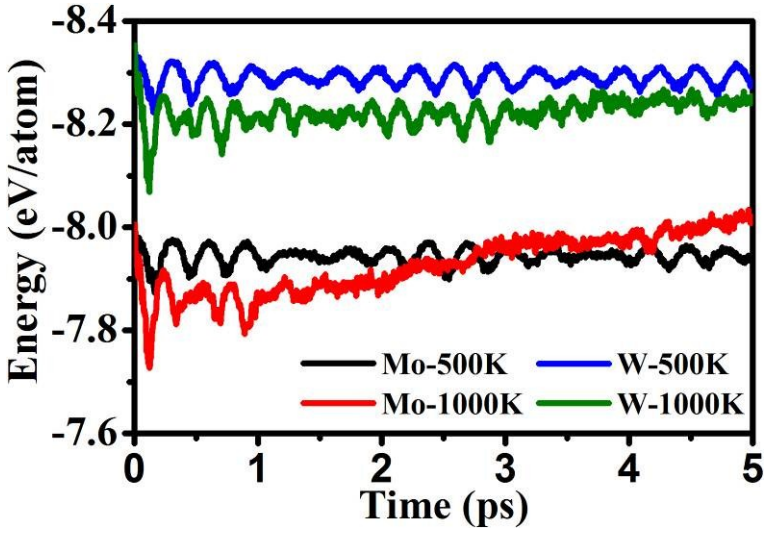

Figure S3. The energy fluctuations with respect to time in AIMD simulations at 500 K and 1000 K for the s-MC_6 monolayers.

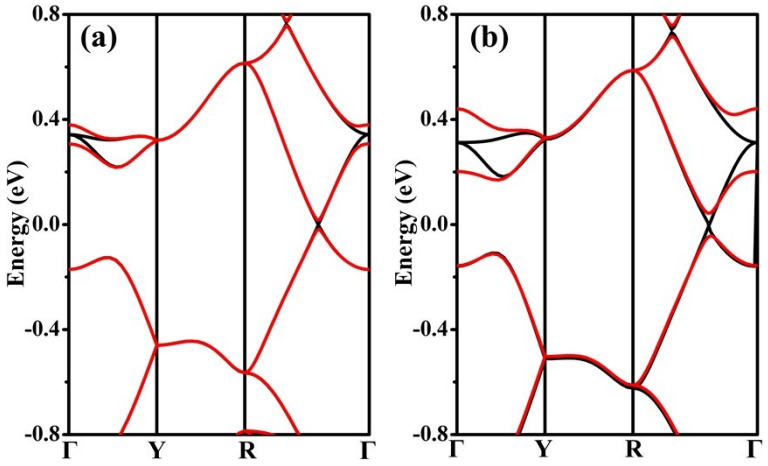

Figure S4. The band structures for (a) s-MoC_6 and (b) s-WC_6 monolayers at the GGA+U level with U = 2.81 eV, J = 0.59 eV and U = 2.67 eV, J = 0.54 eV for Mo and W atom. Red line: with SOC; black line: without SOC. For this case, the band gaps are calculated to be 37 meV and 87 meV for s-MoC_6 and s-WC_6 monolayers, respectively, which are compared to DFT-PBE results (Mo, 35 meV; 89 meV). The calculated topological invariant (Z_2) indicates that MC_6 monolayers are still trivial insulators.

Comp.	Parities of occupied spin-degenerate bands	Product
MoC_6	+ + - - - - + + + - - + - - - + + - + -	Γ (+)
	+ + - - + + + - + - + + - + - - + - + +	
	+ - + + + - - - - - - + + - - + + - - +	
	+ - - + - + + - + - + - - + + - - + + -	M (+)
	- + + - + - - + + - + - - + + - - + - +	
	- + + - + - + - + - + - + - - + - + + -	
WC_6	+ + - - - - + + + - - + - - - + + - + -	Γ (+)
	+ + - + + - - + + - + + - - - + + - + +	
	+ + - - - + - + - - - + + - + - + - - +	
	- + - + - + - + - + - + - + - + - + - +	M (+)
	- + - + - + - + - + - + - + - + - + - +	
	- + - + - + - + - + - + - + - + - + - +	

Figure S5. The parities of occupied bands at Γ (red color) and M (black color) points for MC_6 monolayers. Due to the presence of inversion symmetry in MC_6 monolayers, topological invariant could be directly calculated from the parities of occupied bands at time reversal invariant momenta (TRIM). It yields that the product of Γ and M points are + 1 and + 1 for MC_6 monolayers, which demonstrates the trivial feature of MC_6 structures.

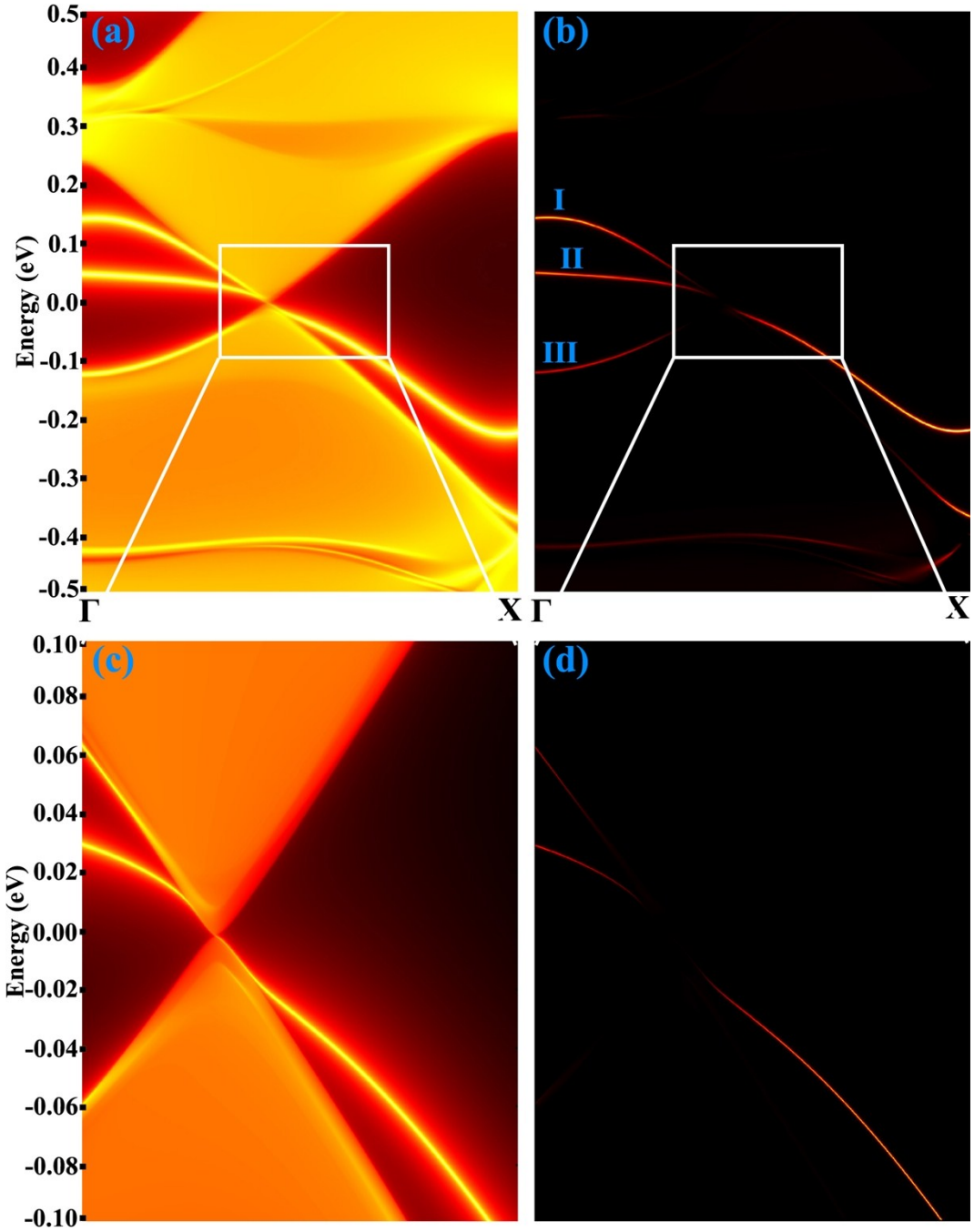

Figure S6. The calculated edge states of semi-infinite lattice for MoC_6 monolayer. The hallmark of 2D topological insulator is the presence of helical gapless edge states. Here, on the basis of maximally localized Wannier functions, we calculate the edge states of a semi-infinite lattice for MoC_6 monolayer constructed by an iterative Green's function method. The upper two edge states (I and II) degenerate into one edge state, which traverse the bulk gap and connect the valence and conduction bands in the vicinity of Fermi level. The edge state (III) just below Fermi level stays in valence-band region. These feathers endow edge states cutting the Fermi level an even number of times, further supporting the trivial nature in the MoC_6 monolayer.

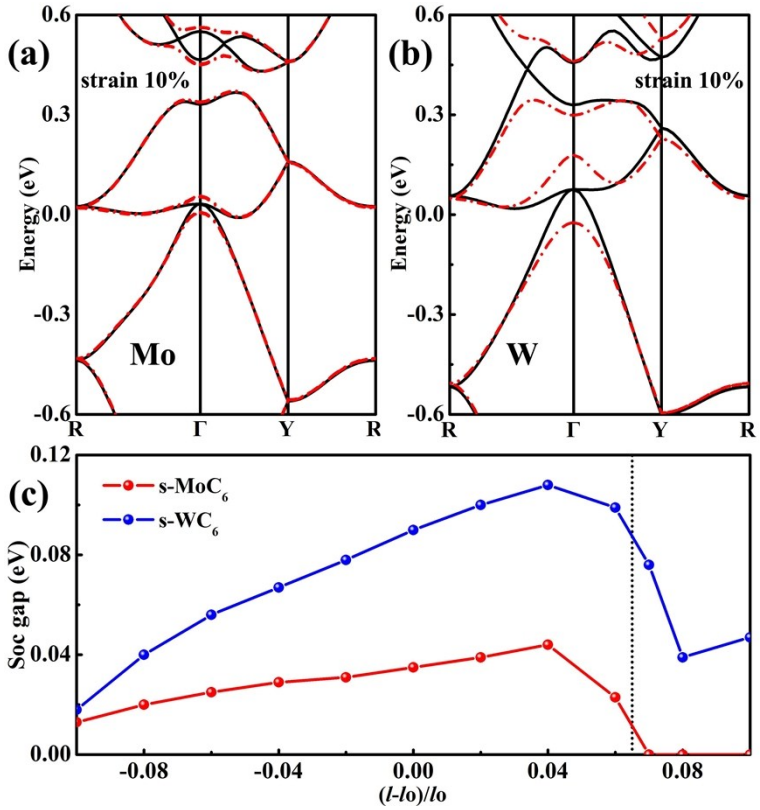

Figure S7. (a) Selected band structures for (a) s-MoC_6 and (b) s-WC_6 monolayers under strain 10% with (red) and without (black) SOC. (c) The SOC-induced gaps of s-MC_6 monolayers as a function of applied external biaxial strain, obtained with PBE + SOC.

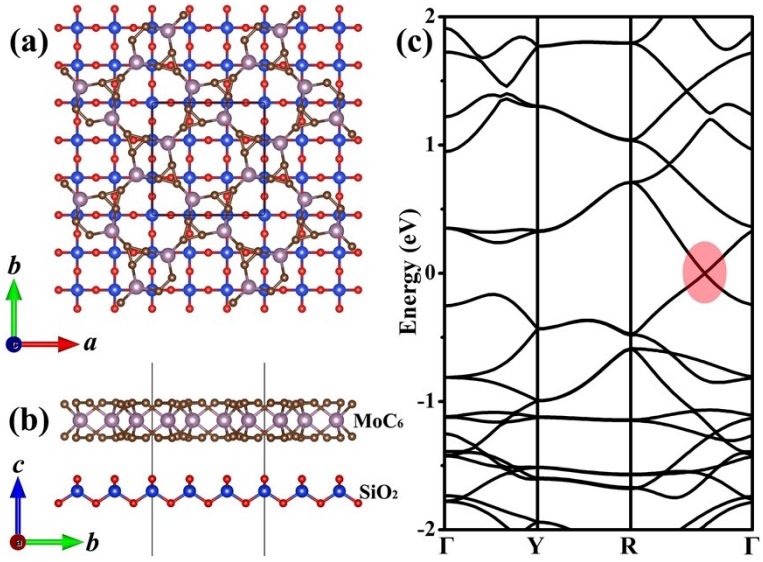

Figure S8. Crystal structure of s-MoC_6 grown on a SiO_2 substrate from the (a) top and (b) side view. (c) The band structure for s-MoC_6@SiO_2.