Electronic Supplementary Information

Square transition-metal carbides $\text{MC}_6$ ($\text{M} = \text{Mo, W}$) as stable two-dimensional Dirac cone materials

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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-MC₆ monolayers.

Figure S4. The band structures for (a) s-MoC₆ and (b) s-WC₆ 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-MoC₆ and s-WC₆ monolayers, respectively, which are compared to DFT-PBE results (Mo, 35 meV; 89 meV). The calculated topological invariant (Z₂) indicates that MC₆ monolayers are still trivial insulators.
**Figure S5.** The parities of occupied bands at $\Gamma$ (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 $\Gamma$ 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$_2$. 