Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

Supporting Information

Direct Tuning of Large-Gap Quantum Spin Hall Effect in Mono-Transition Metal Carbide MXenes

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Supporting information consists of 5 Figures (Figure S1-S7) and 2 Tables (Table S1-S2).

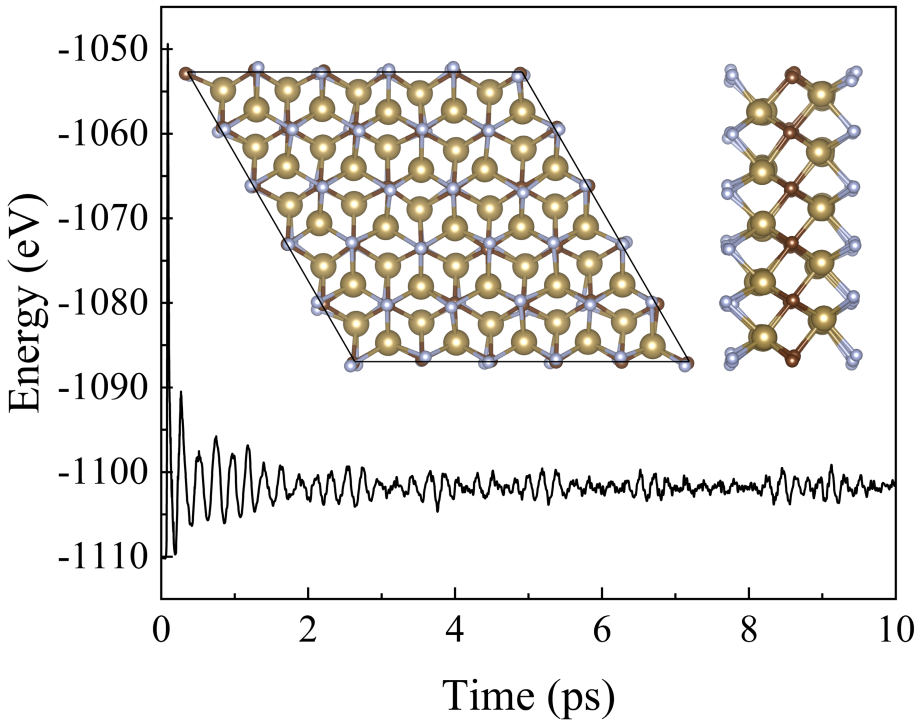

Figure S1. Fluctuations of total energies of Ta_2CF_2 monolayer and a snapshot of the equilibrium structure at the end of 10 ps MD simulations at the temperature of 500 K.

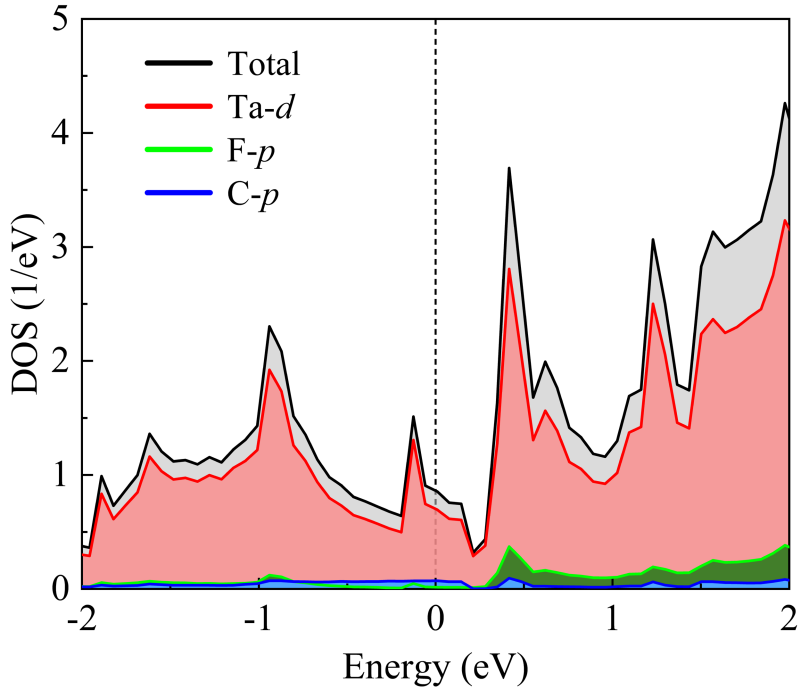

Figure S2. The projected partial densities of states (PDOS) of atoms orbitals with SOC by using the PBE functionals.

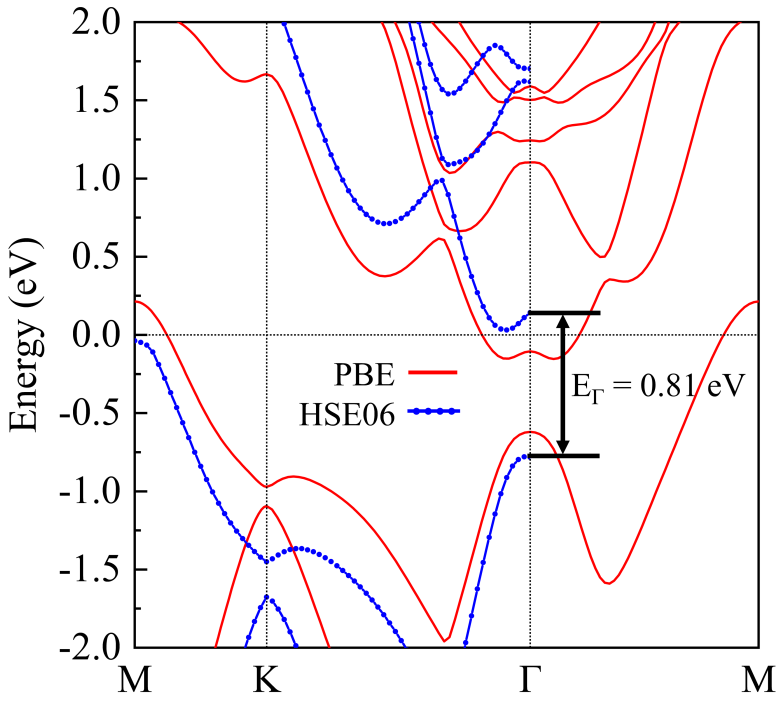

Figure S3. Band structure for Ta_2CF_2 monolayer calculated with SOC by using the PBE (red lines) and HSE06 (blue lines) functionals.

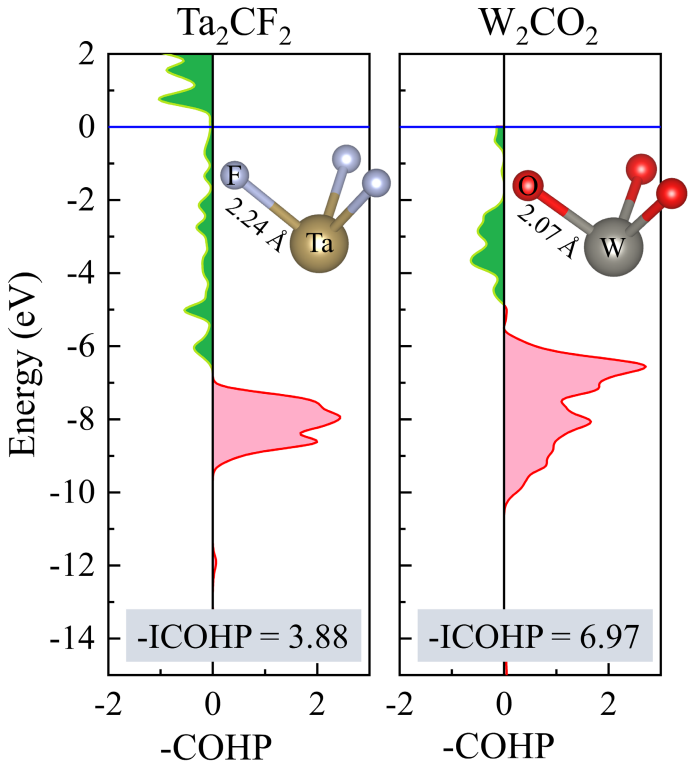

Figure S4. The −COHP and −ICOHP values for chemical bonds in the Ta_2CF_2 and W_2CO_2 monolayer. The pink color corresponds to bonding states, and green color corresponds to antibonding states.

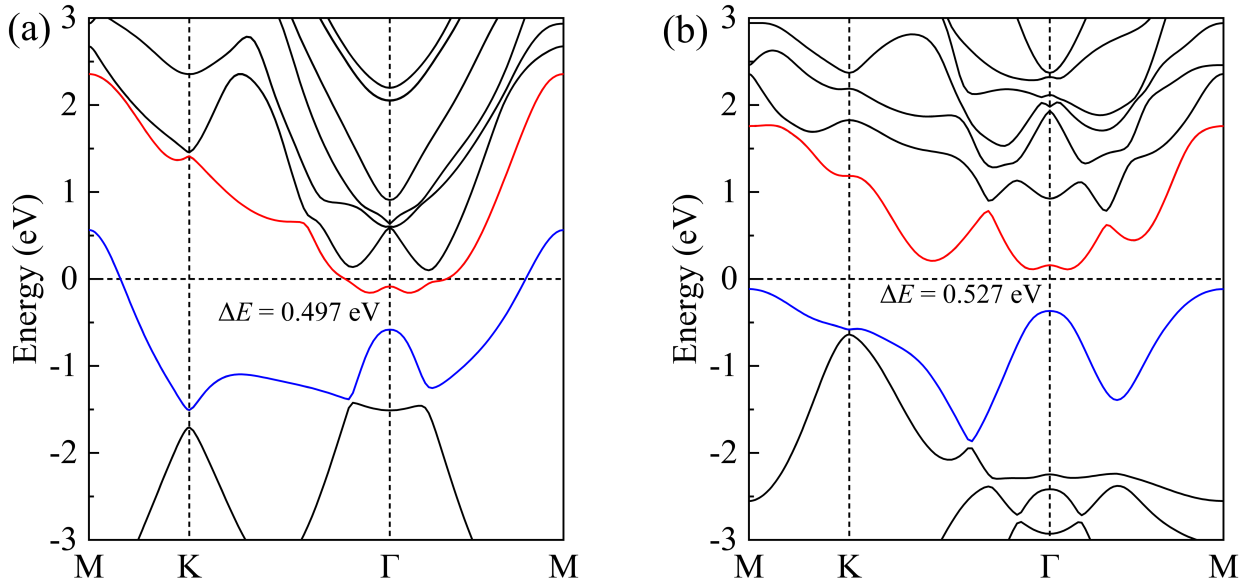

Figure S5. The electronic band structures of Ta_2CF_2 monolayer under the thickness (Δh) of 4.79 Å (a) and 6.39 Å (b) between F and F atoms, respectively.

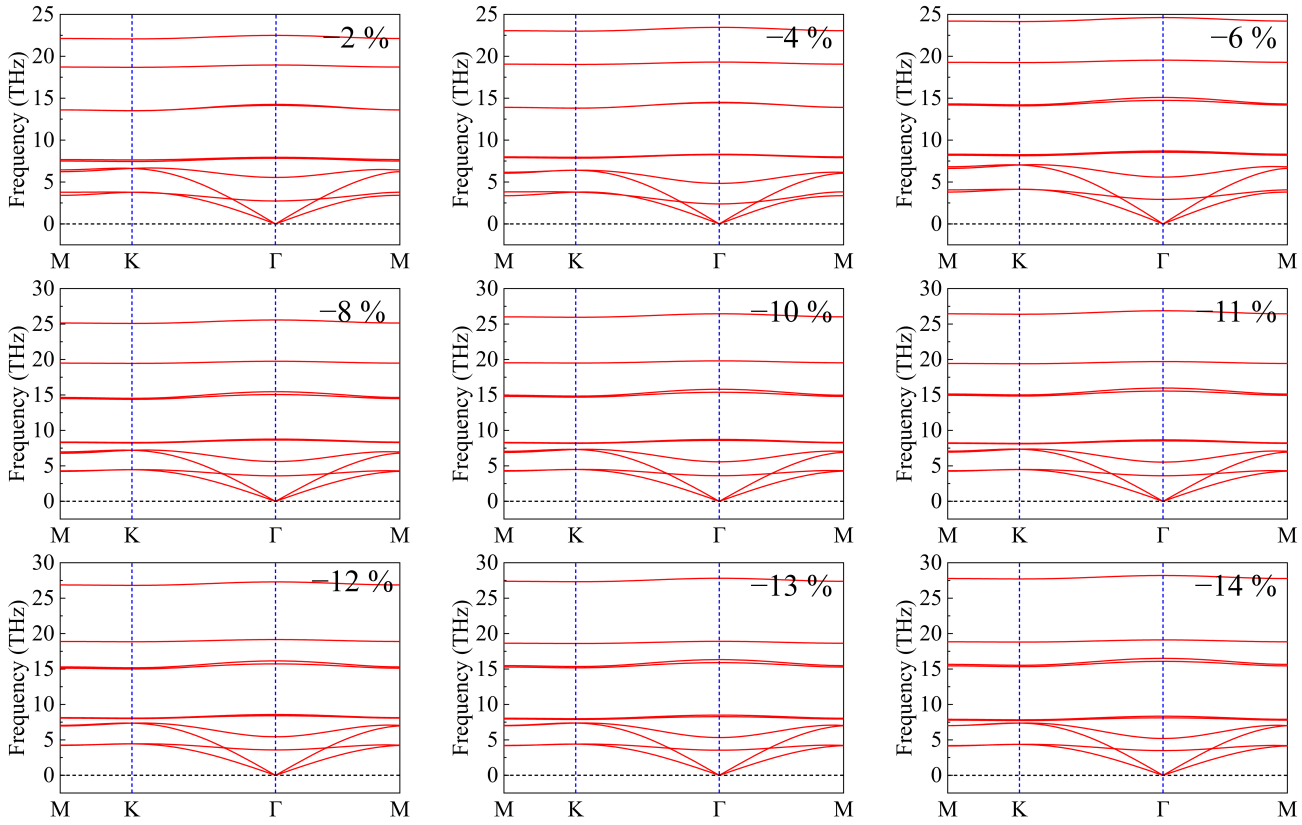

Figure S6. The phonon spectrum of Ta_2CF_2 monolayer under different hydrostatic strains (the compressing of the lattice from 2% to 14%).

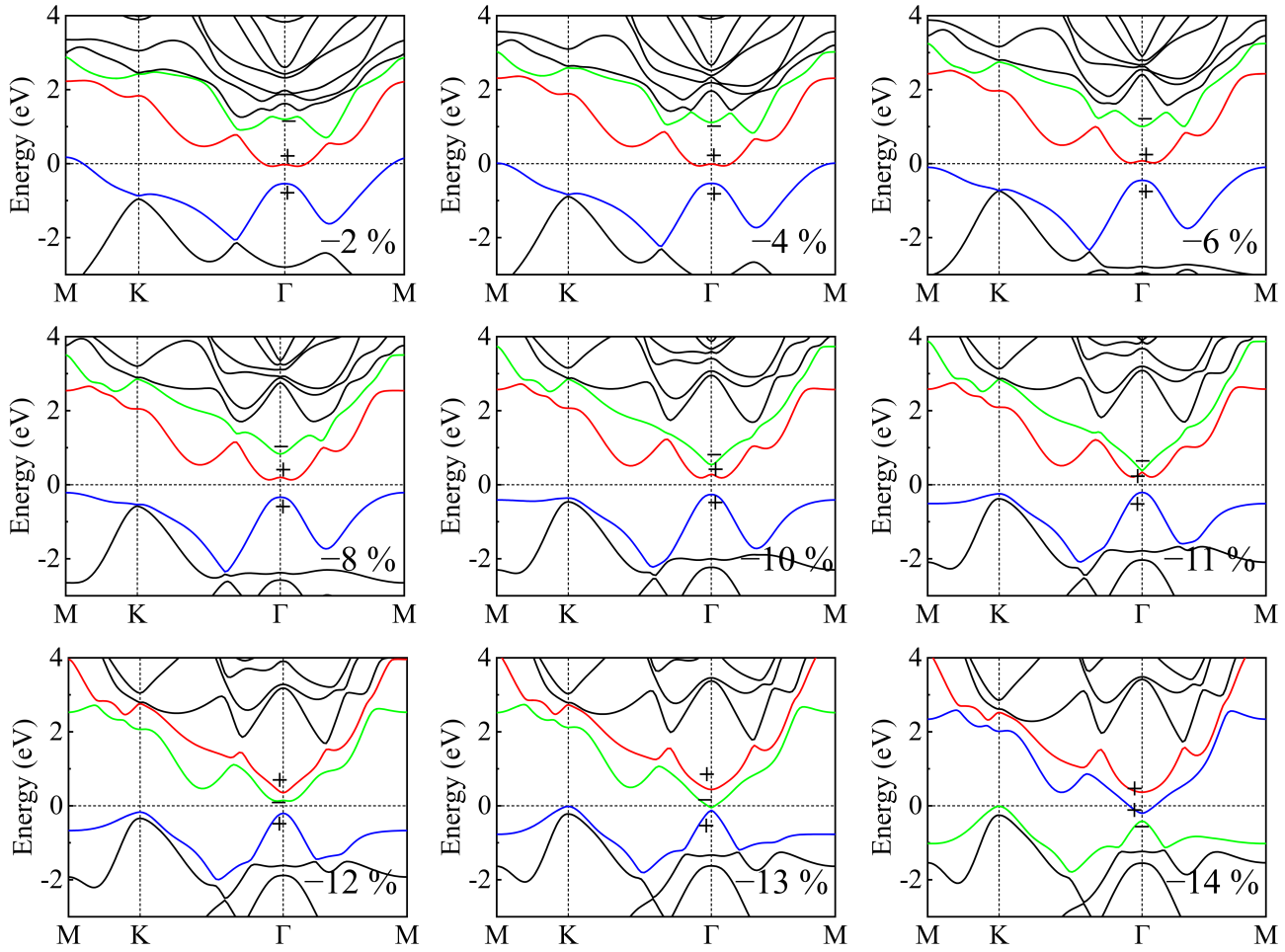

Figure S7. The electronic band structures of Ta_2CF_2 monolayer under different hydrostatic strains by using the PBE functionals (the compressing of the lattice from 2% to 14%), the evolution for the relative parameters is shown in Table S2. Parities of the Bloch states at the Γ-point are denoted by +, −.

Table S1. In different GGA+*U* studies, the nontrivial gaps at the Γ-point (E_Γ) under the thickness (Δh) of 4.79 Å, 5.59 Å and 6.39 Å, respectively.

Δh	$U = 0$	$U = 1$	$U = 2$
4.79 Å	0.497 eV	0.533 eV	0.573 eV
5.59 Å	0.515 eV	0.564 eV	0.631 eV
6.39 Å	0.527 eV	0.597 eV	0.687 eV

Table S2. Lattice parameters (a), thickness of F and F atoms (Δh), nontrivial gaps at the Γ-point (E_Γ), and $\mathbb{Z}_2$ topological invariants for the Ta_2CF_2 monolayer under different hydrostatic strains. The values of E_Γ calculated using the PBE functional.

Strains (%)	a (Å)	Δh (Å)	E_Γ (eV)	$\mathbb{Z}_2$
0	2.97	5.59	0.515	1
−2	2.91	5.66	0.518	1
−4	2.85	5.74	0.523	1
−6	2.79	5.83	0.528	1
−8	2.73	5.92	0.536	1
−10	2.68	6.02	0.546	1
−11	2.65	6.07	0.551	1
−12	2.62	6.12	0.353	1
−13	2.59	6.18	0.074	1
−14	2.56	6.24	0.211	0