Supporting Information of

High negative Poisson's ratio in a flexible two-dimensional Tungsten Carbide monolayer

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Section S1. Description of surface functionalized W_2C

As reported, the MXene materials are usually produced by selective etching the A element layer from parent layered MAX phases employing strong HF solutions and the intrinsic MXenes possess high hydrophilic nature.[1] Thus, the synthesis process would inevitably lead to the incomplete or mixed F, O and OH functional groups presenting on their surface, which may affect their configurations and performances.[1, 2] In fact, numerous researchers have reported that these terminations could tune various properties of the intrinsic MXenes including mechanical, electronic, magnetic, and energy storage capacity, etc.[2-6] Hence, surface functionalized W_2C MXene, W_2CT_2 (T = O, F and OH), are also investigated. The most stable configurations of these W_2CT_2 are displayed in Figure S2. Apparently, the three functionalized groups lie at completely different position on the both sides of W_2C sheet. F atoms are located on the top of the side W atoms, O atoms prefer to stay above the top sites of the middle C atoms, and OH groups stabilize above the hollow site consist of three neighboring C atoms, which are in good accordance with the previous work.[3, 5] Formation energies (Table S1) and phonon spectrums (Figure S1) demonstrate the functionalized W_2CO_2, W_2CF_2, and $W_2C(OH)_2$ are stable in both thermodynamics and kinetics.

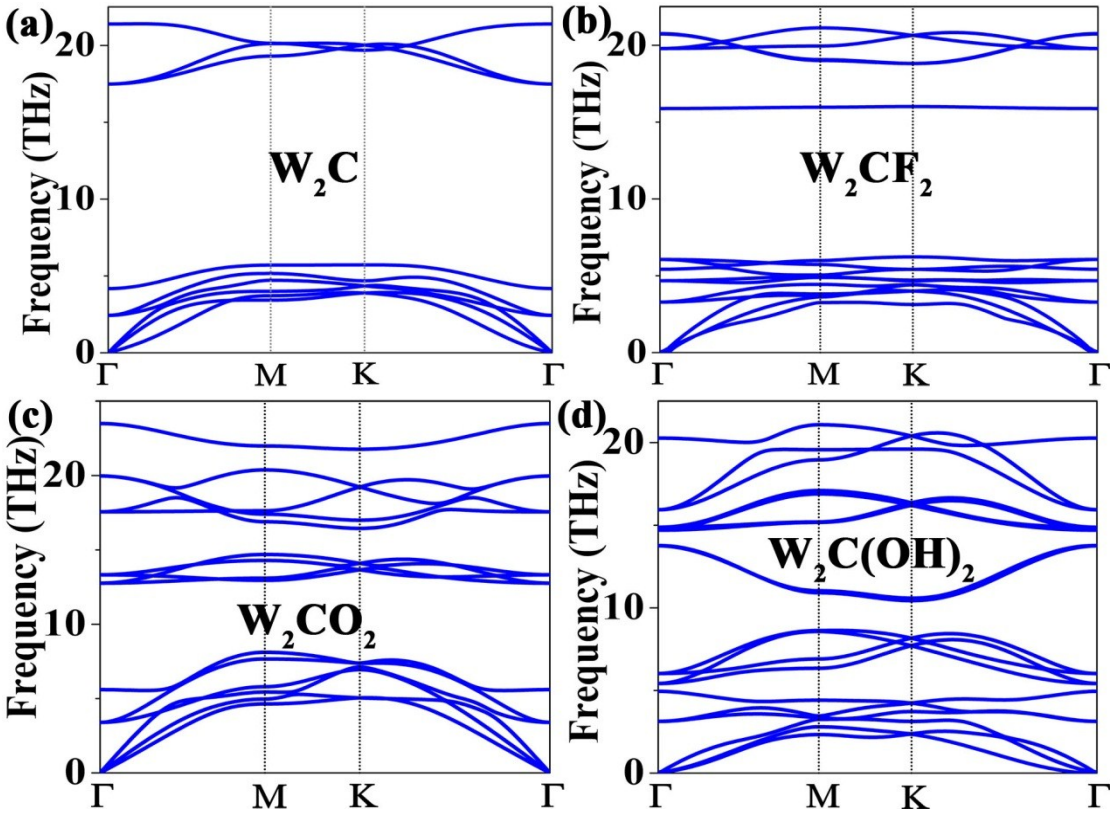

Figure S1. Phonon spectra of the strain-free (a) W_2C, (b) W_2CF_2, (c) W_2CO_2, and (d) $W_2C(OH)_2$.

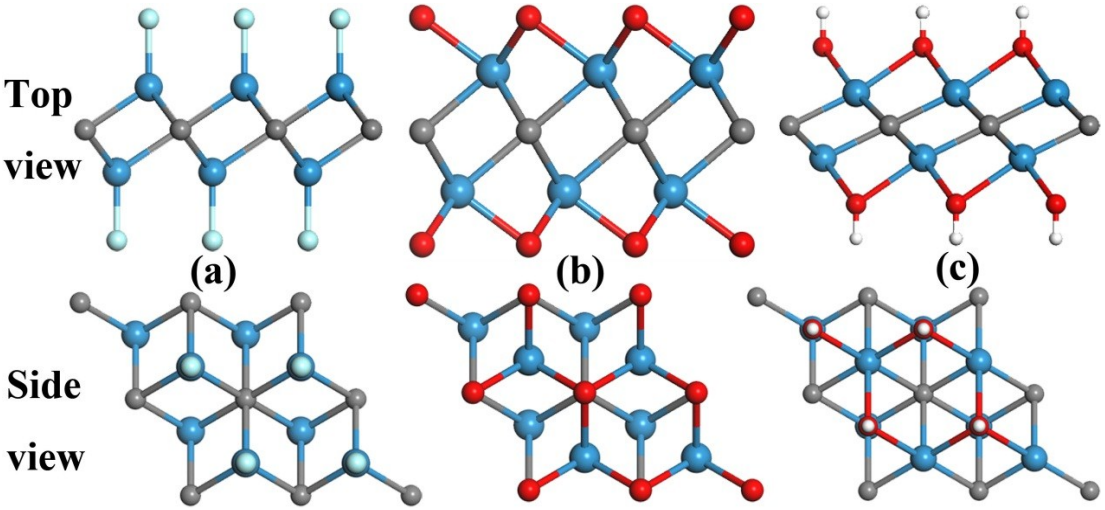

Figure S2. Top and side views of the most stable configurations for (a) W_2CF_2, (b) W_2CO_2, and (c) $W_2C(OH)_2$.

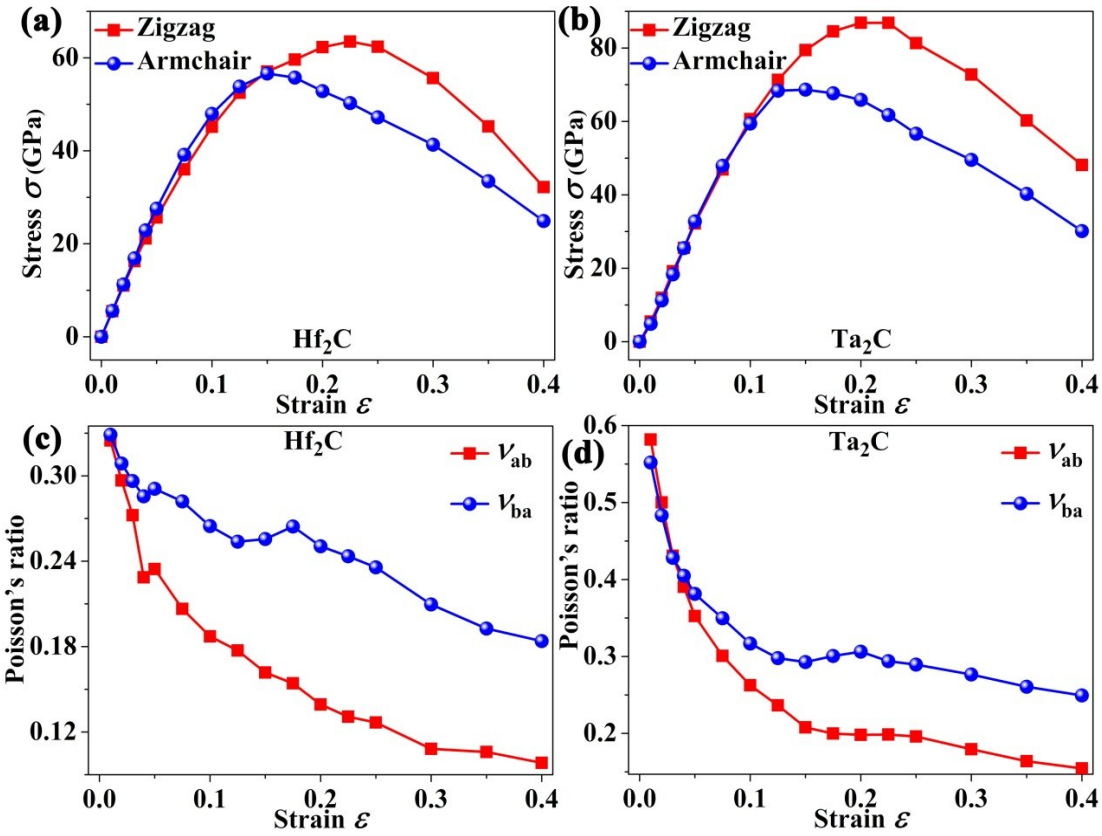

Figure S3. Stress–strain curves of (a) Hf_2C and (b) Ta_2C under uniaxial stretching, together with the corresponding Poisson's ratios of (c) Hf_2C and (d) Ta_2C.

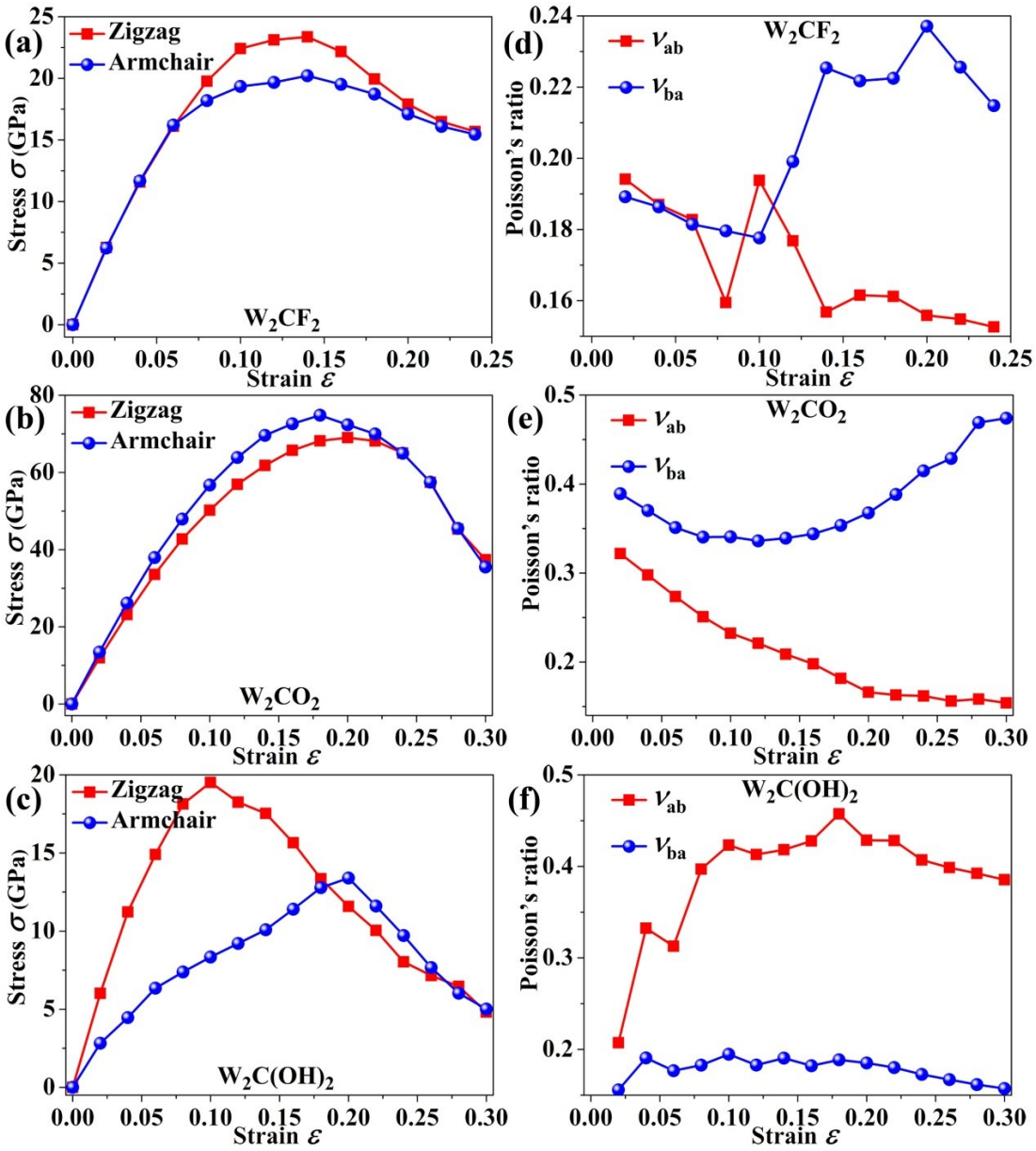

Figure S4. Stress–strain curves of W_2CT_2: (a) W_2CF_2, (b) W_2CO_2, (c) $W_2C(OH)_2$, and the corresponding Poisson's ratios of (d) W_2CF_2, (e) W_2CO_2, (f) $W_2C(OH)_2$.

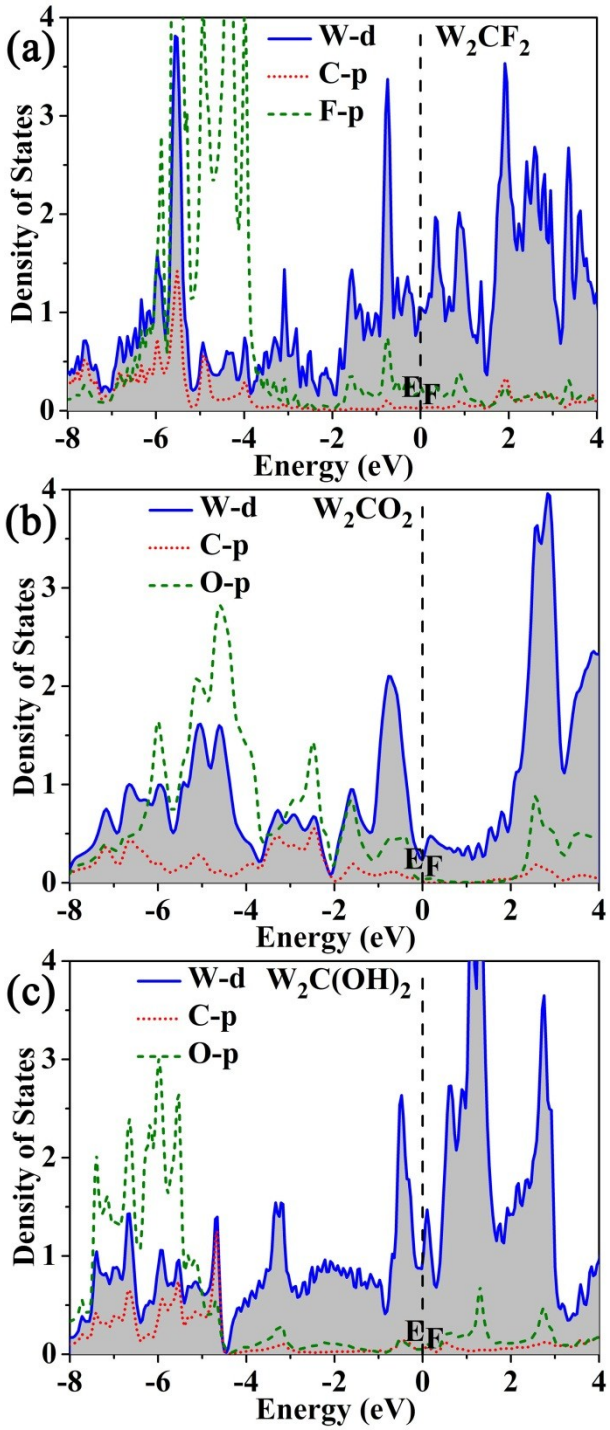

Figure S5. The projected DOS of W_2CT_2: (a) W_2CF_2, (b) W_2CO_2, and (c) $W_2C(OH)_2$.

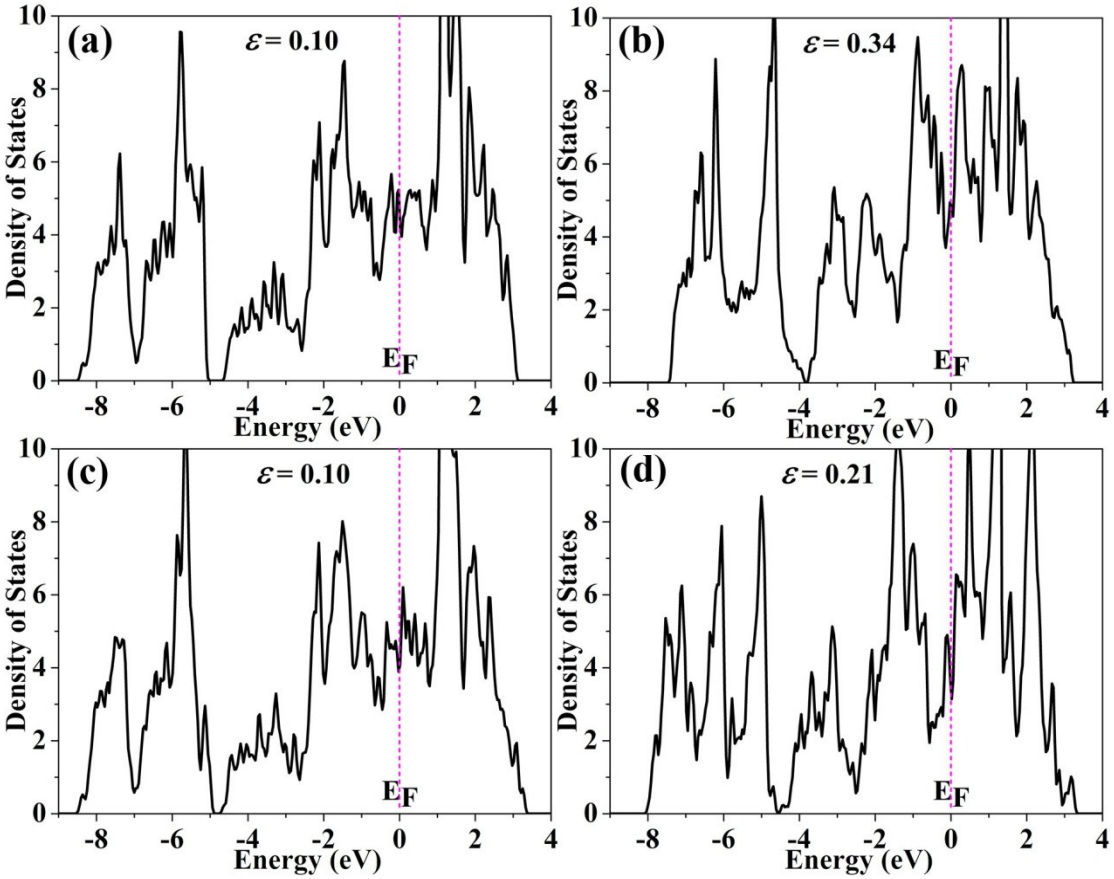

Figure S6. The total DOS of the strained W_2C: uniaxial tension along the zigzag direction of (a) 0.10 and (b) 0.34, as well as along the armchair direction of (c) 0.10 and (d) 0.21.

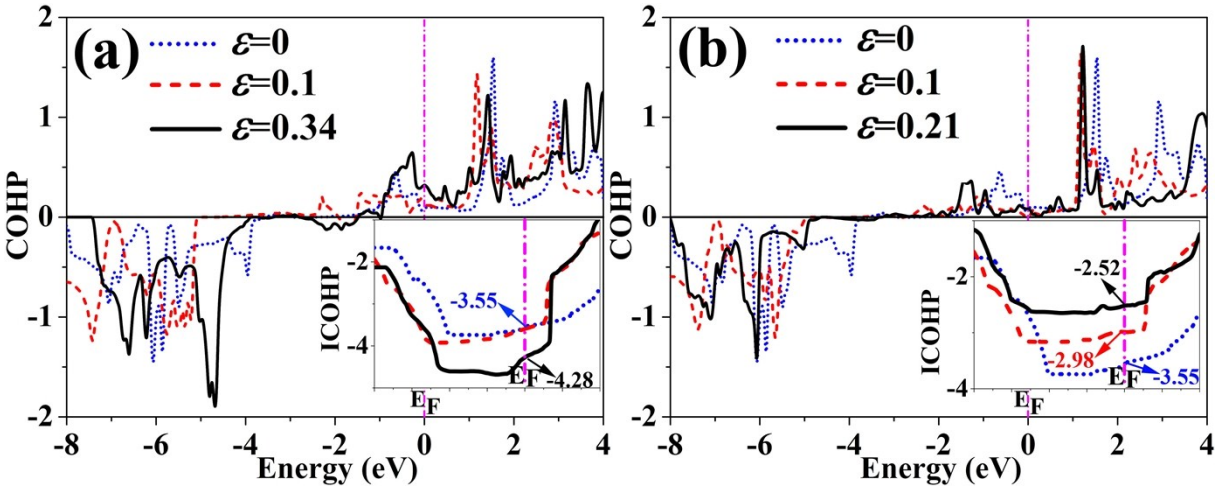

Figure S7. COHP curves of W-C bonds and their corresponding integrals (inserts) under uniaxial tension along the zigzag (a) and armchair (b) directions.

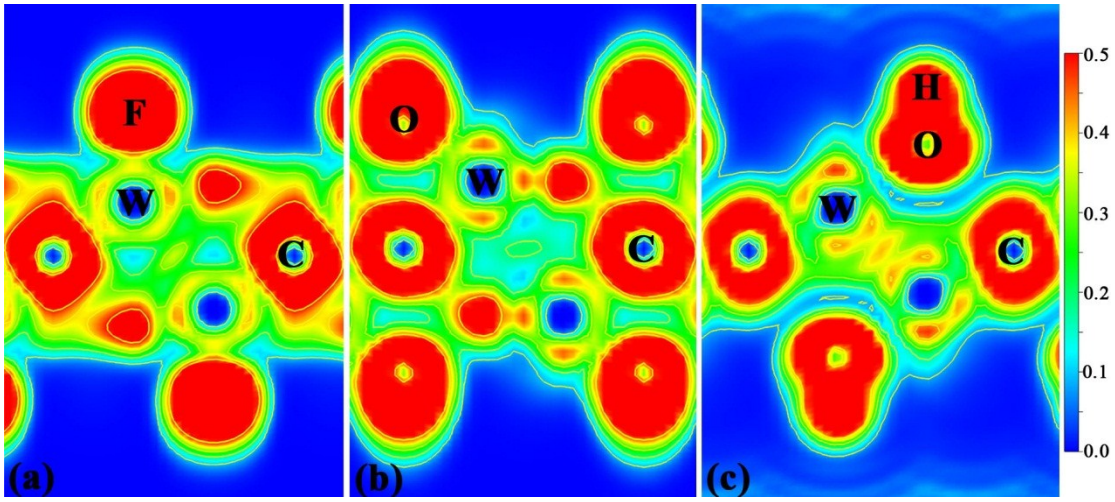

Figure S8. ELF maps of the section made up of C atoms, metal atoms and terminal groups: (a) W_2CF_2, (b) W_2CO_2, and (c) $W_2C(OH)_2$.

Table S1 The formation energies (E_f) of intrinsic W_2C and the surface functionalized W_2CT_2(T=F, O, and OH.

Species	W_2C	W_2CF_2	W_2CO_2	$W_2C(OH)_2$
E_f (eV)	-4.90	-7.76	-9.66	-8.72

References

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