Supporting Information

Janus MXene nanosheets with strain-induced reversible magnetic state transition for storing information without electricity

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Table S1. The elastic constant (C), Young's modulus (Y), shear modulus (G), and Poisson ratio (υ) of Janus TiVC MXene. (unit: N/m)

	C_{11}	C_{12}	C_{66}	Y	G	υ
TiVC	55.67	3.55	26.06	55.44	26.06	15.68

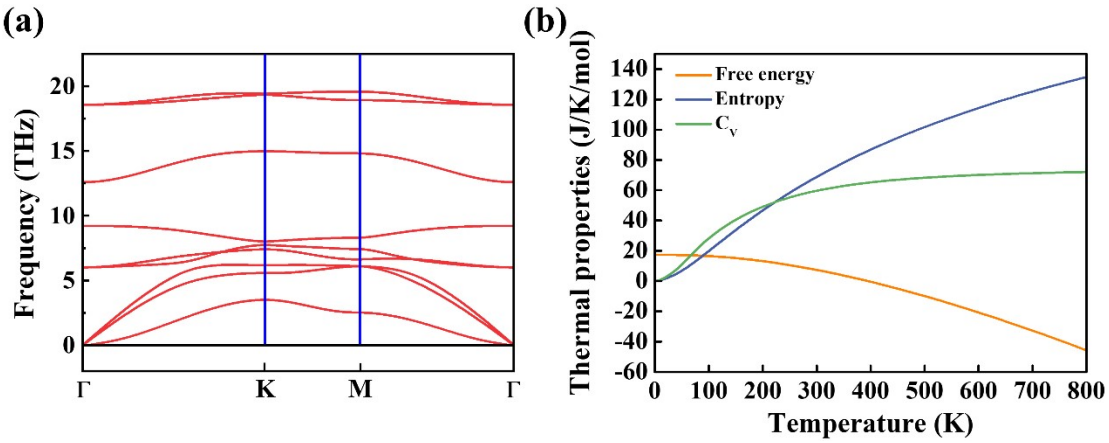

Fig. S1. The (a) Phonon dispersions and (b) thermal properties of Janus TiVC MXene.

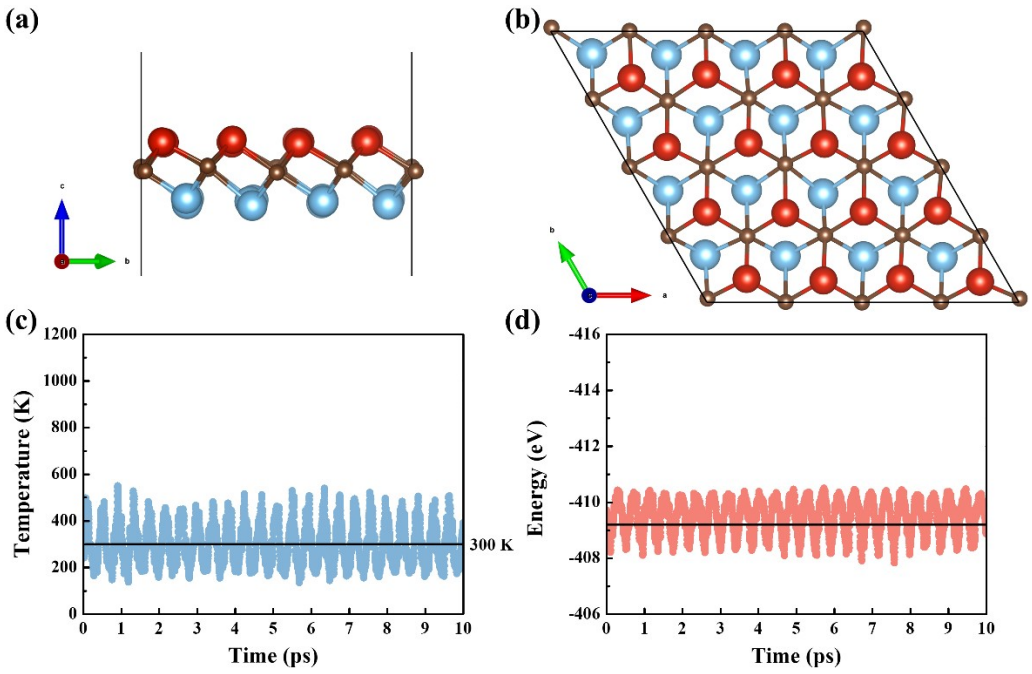

Fig. S2. The (a) side view and (b) top view of TiVC monolayer structure after 10 ps AIMD simulation. The curves of (c) temperature and (d) energy over time.

For Janus TiVC MXene monolayer, we investigated its dynamic stability using the ab initio molecular dynamics (AIMD) method, as shown in the Fig. S3. And besides, for intrinsic TiVC, the V-C bond length of $d_{V\text{-}C}$ is 2.000 Å and the Ti-C bond length of $d_{Ti\text{-}C}$ is 2.153 Å. After AIMD simulation, the average $d_{V\text{-}C}$ is 2.023 Å and the average $d_{Ti\text{-}C}$ is 2.124 Å. The TiVC bond length undergoes minimal changes, and TiVC monolayer structure remains intact. The structures of TiVC monolayer after AIMD simulation are shown in Fig. S3(a) and S3(b). Additionally, during the AIMD process, we employed the NVT ensemble, and as such, temperature and energy fluctuated within a specific range throughout the simulation, as shown in Fig. S3(c) and S3(d). The results show that the structure of TiVC monolayer will not change greatly at room temperature after 10 ps AIMD simulation. The thermodynamic and dynamics stability of TiVC monolayer shows that it can exist in nature.

During the AIMD simulation, the Verlet algorithm is used to solve the ions' equations of motion. The total simulation time is set to 10 ps, with a time step of 2 fs, resulting in a total of 5,000 ion steps. The temperature control of the system was implemented using the built-in Nosé-Hoover thermostat provided in the VASP. Throughout the entire AIMD simulation process, Brillouin zone integration was restricted solely to the Γ-point.

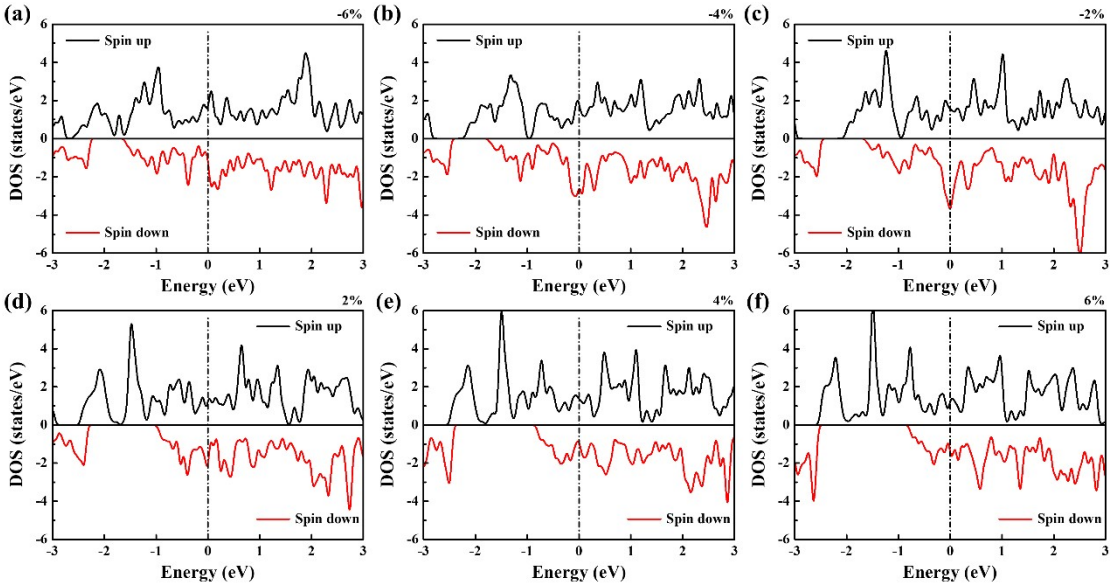

Fig. S3. The DOS of Janus TiVC MXene under different strain.

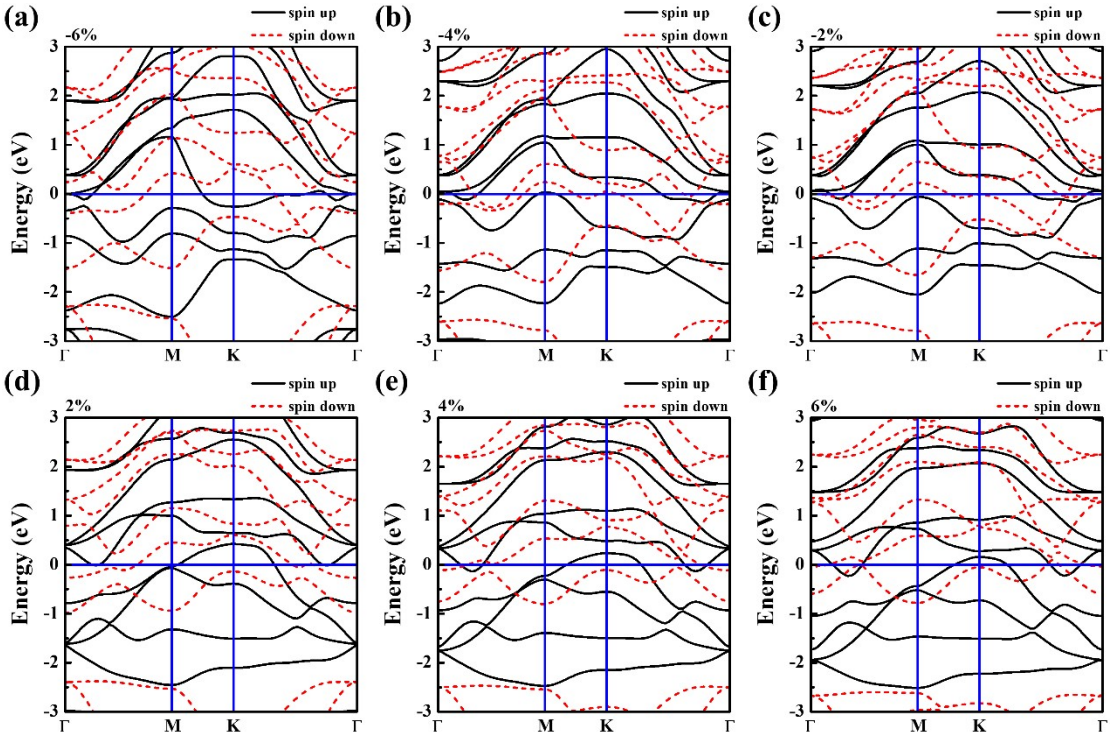

Fig. S4. The band structure of Janus TiVC MXene under different strain.

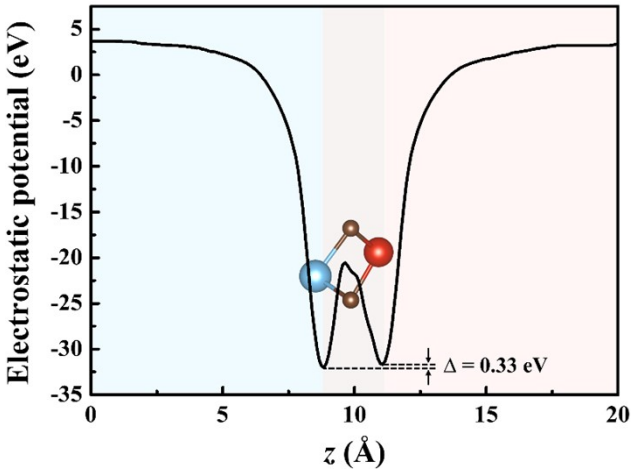

Fig. S5. The electrostatic potential of Janus TiVC MXene.

Table S2. The lattice parameters, magnetic moments and magnetic ground state (MGS) of Janus TiVC MXene.

Strain	$a = b$ (Å)	M_{Ti} (μ_B)	M_V (μ_B)	M_{tot} (μ_B)	MGS
-6%	2.815	0.915	-0.826	0.089	A-AFM
-4%	2.875	0.869	-0.813	0.056	A-AFM
-2%	2.935	0.845	-0.785	0.06	A-AFM
0%	2.995	0.645	-0.186	0.459	A-AFM
2%	3.055	0.154	2.115	2.269	FM
4%	3.115	0.635	2.033	2.668	FM
6%	3.175	0.385	2.181	2.566	FM

The key energy data of intrinsic TiVC monolayer:

Table S3. The absolute energies (E) of TiVC under different magnetic configurations. ΔE represents the difference between magnetic energy and nonmagnetic energy.

	NM	FM	A-AFM	C-AFM	G-AFM
E (eV)	-18.91	-23.11	-23.11	-19.22	-23.05
ΔE (eV)	-	-4.20	-4.20	-0.31	-4.14

The geometric parameters of intrinsic TiVC monolayer (POSCR file):

TiVC

1.00000000000000

2.5935654310000000 -1.4973957000000000 0.0000000000000000

0.0000000000000000 2.9947914000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

C Ti V

1 1 1

Direct

0.0000000000000000 0.0000000000000000 0.5046294830732109

0.3333333333333357 0.6666666666666643 0.4405021374672496

0.6666666666666643 0.3333333333333357 0.5548683794595396

Table S4. The gain and loss of single Ti, V, and C atom with different tensile strains (unit: *e*), as well as, the dipole moment of Janus TiVC MXene (unit: Debye).

Strain	Ti	V	C	dipole moment
-6%	-0.943	-0.957	1.900	0.037
-4%	-0.990	-0.956	1.947	0.031
-2%	-1.021	-0.972	1.993	0.032
0%	-1.061	-1.010	2.071	0.054
2%	-1.164	-1.007	2.171	-0.110
4%	-1.172	-0.964	2.136	-0.118
6%	-1.232	-0.972	2.205	-0.122