First principles study on magnetism in some novel MXene materials

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Table S1 The calculated lattice constants, total energies (eV) and atomic magnetic moment for the metal atoms (μB/atom) of 1H and 1T type M_2C (M=Sc, Ti, Fe, Co, Ni, Cu, Zn) MXenes in AFM, FM and NM configurations, and the ground energy configuration are highlighted in bold-typeface.

			a (Å)	*E* (eV)	Magnetization				*a* (Å)	*E* (eV)	Magnetization
Sc_2C	1H	AFM	3.283	−37.290	0.328	Ti_2C	1H	AFM	3.042	−40.715	0.812
		FM	3.281	−37.298	0.389			FM	3.042	−40.702	0.521
		NM	3.251	−37.077				NM	3.042	−40.429	
	1T	AFM	3.339	−38.386	0.213		1T	**AFM**	**3.038**	**−42.060**	**0.629**
		FM	3.341	−38.415	0.422			FM	3.059	−42.009	0.488
		NM	3.322	−38.290				NM	3.022	−41.759	
Fe_2C	1H	AFM	2.622	−42.537	1.902	Co_2C	1H	AFM	2.540	−41.210	1.349
		FM	2.602	−43.014	2.192			**FM**	**2.562**	**−41.313**	**1.260**
		NM	2.522	−42.271				NM	2.464	−40.677	
	1T	AFM	2.833	−43.476	2.223		1T	AFM	2.824	−41.135	1.049
		FM	**2.794**	**−43.528**	**2.077**			FM	2.875	−41.075	0.998
		NM	2.857	−41.917				NM	2.865	−40.738	
Ni_2C	1H	NM	2.584	−39.015		Cu_2C	1H	**NM**	**2.700**	**−35.9165**	
	1T	**NM**	**2.899**	**−39.453**			1T	NM	2.905	−35.75592	
Zn_2C	1H	NM	3.035	−32.177							
	1T	**NM**	**3.471**	**−32.992**							

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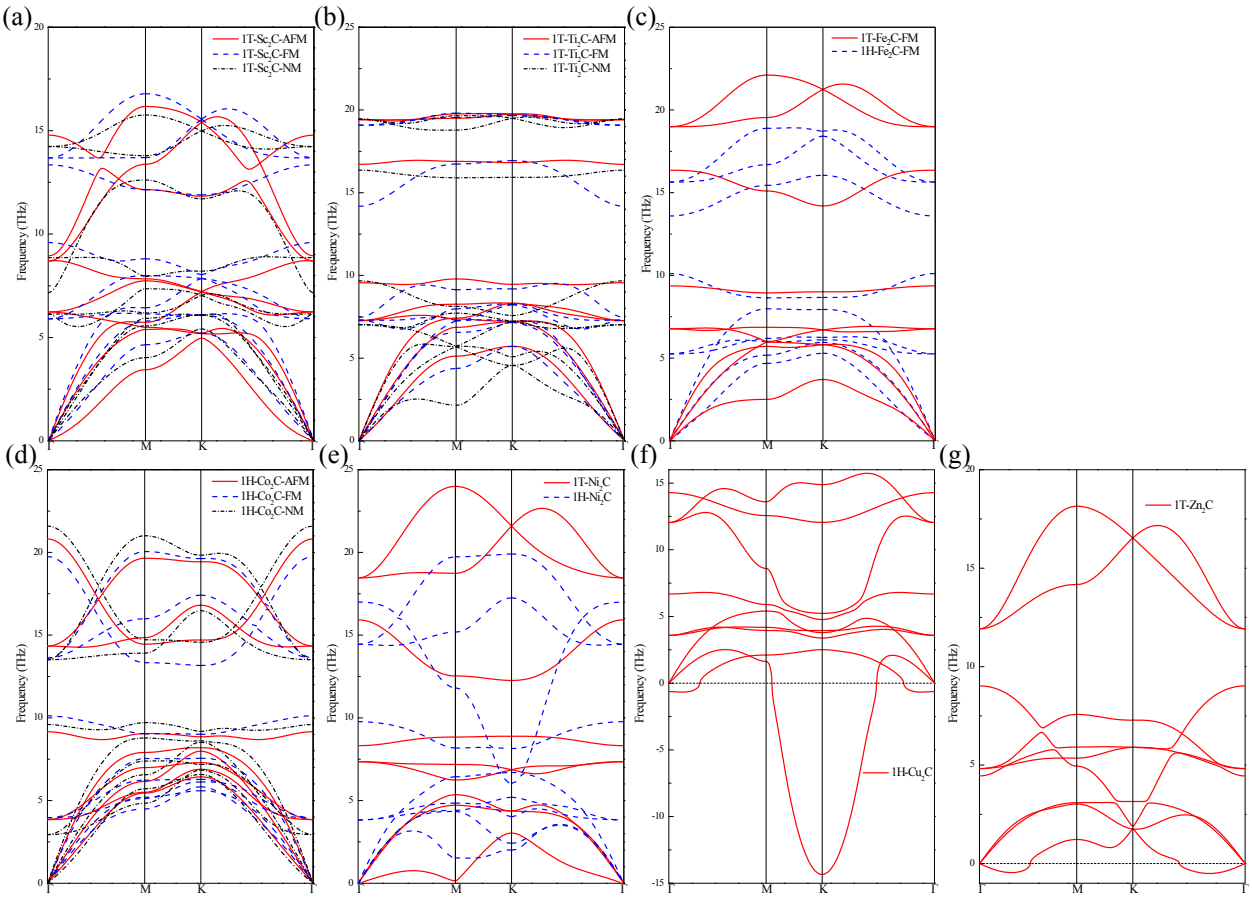

Fig. S1 The phonon dispersions of Sc_2C (a), Ti_2C (b), Fe_2C (c), Co_2C (d), Ni_2C (e), Cu_2C (f) and Zn_2C (g) MXenes along the high symmetry points Γ(0, 0, 0)→M(½, 0, 0)→K(⅓, ⅓, 0)→Γ(0, 0, 0) of the Brillouin zone.

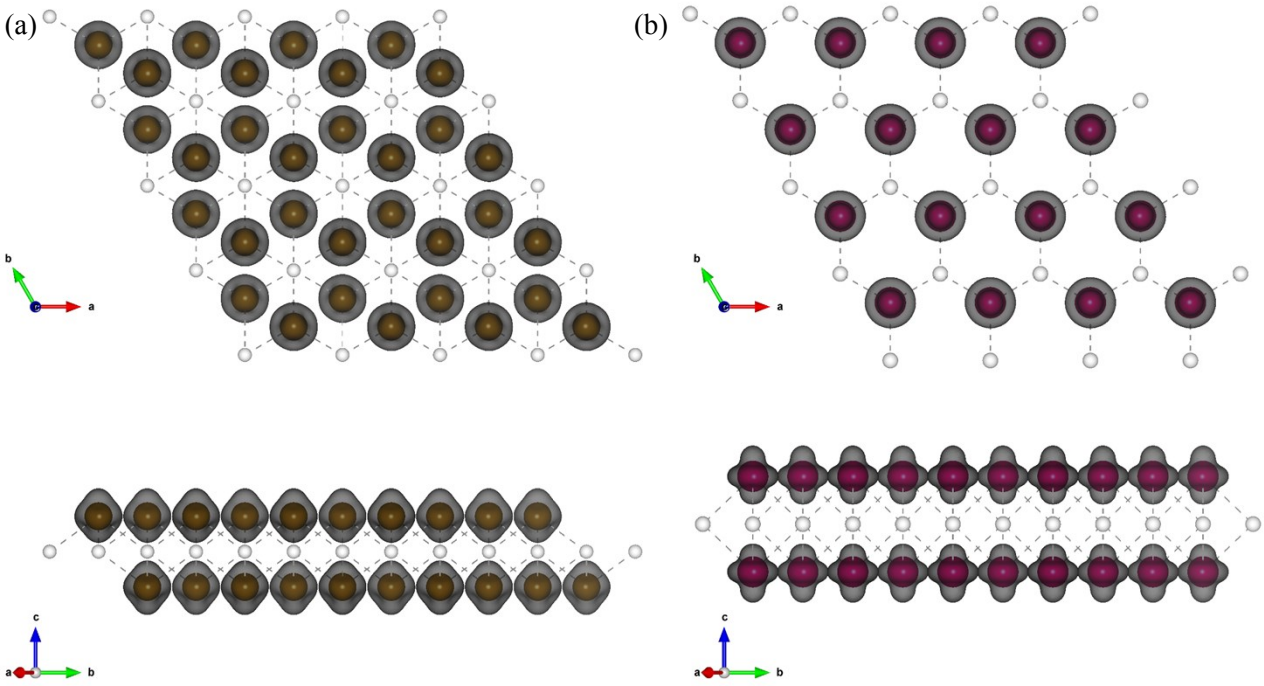

Fig. S2 Top and side view of the spin charge density distribution of the FM magnetic configuration 1T-Fe_2C (a) and 1H-Co_2C (b).

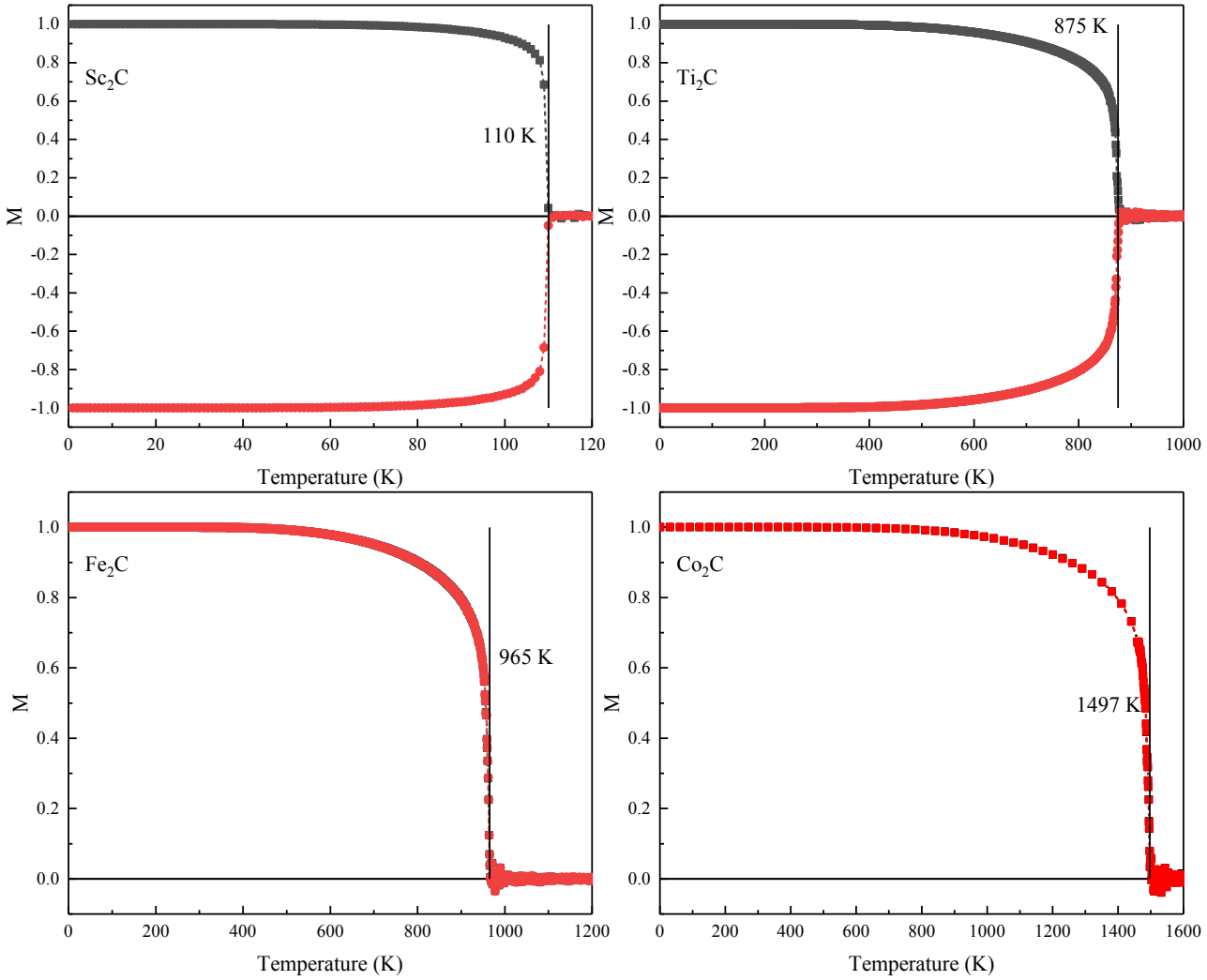

Fig. S3 Average magnetization orientation as a function of temperature for magnetic 1T-Sc_2C (a), 1T-Ti_2C (b), 1T-Fe_2C (c) and 1H-Co_2C (d) MXenes from Monte Carlo simulations.