

First-Principles Study on Magnetic MXenes for Free Radicals

Trapping and Sensing

Table S1 Formation energies of proposed MXenes

MXenes	$E_f(\text{eV/f.u.})$	MXenes	$E_f(\text{eV/f.u.})$
Fe_2CO_2	-1.57	Co_2CO_2	-0.14
Fe_2CF_2	-4.40	Co_2CF_2	-3.47
Fe_2CCl_2	-0.92	Co_2CCl_2	-0.19
Fe_2CBr_2	0.02	Co_2CBr_2	0.68
Ni_2CO_2	1.01	Mn_2CO_2	-3.40
Ni_2CF_2	-3.19	Mn_2CF_2	-5.66
Ni_2CCl_2	0.45	Mn_2CCl_2	-1.88
Ni_2CBr_2	1.31	Mn_2CBr_2	-0.80

Table S2 Effect of supercell size on the minimum radical-radical separation distance, adsorption energy, adsorption bond length and total magnetic moment.

Supercell Size	Adsorption Coverage	Min. Radical-Radical Distance (Å)	Adsorption Energy (eV)	Adsorption Bond Length (Å)	Magnetic Moment (μ_B)
2×2×1	25.0%	5.92	-2.01	1.43	2.01
3×3×1	11.1%	8.89	-2.51	1.45	2.01
4×4×1	6.25%	11.84	-2.94	1.46	2.01

Table S3 Convergence of SHC for Fe₂CF₂ as a function of k-mesh density. $\Delta\text{SHC} = |\text{SHC}_N - \text{SHC}_{N-1}|$ represents the absolute difference between successive k-meshes.

K-mesh	SHC ($\times 10^4(\hbar/e) \cdot \text{S/m}$)	ΔSHC ($\times 10^4(\hbar/e) \cdot \text{S/m}$)
10 \times 10 \times 1	19.44	-
20 \times 20 \times 1	14.21	5.23
30 \times 30 \times 1	20.57	6.36
50 \times 50 \times 1	8.60	11.97
100 \times 100 \times 1	9.10	0.50
200 \times 200 \times 1	9.72	0.38

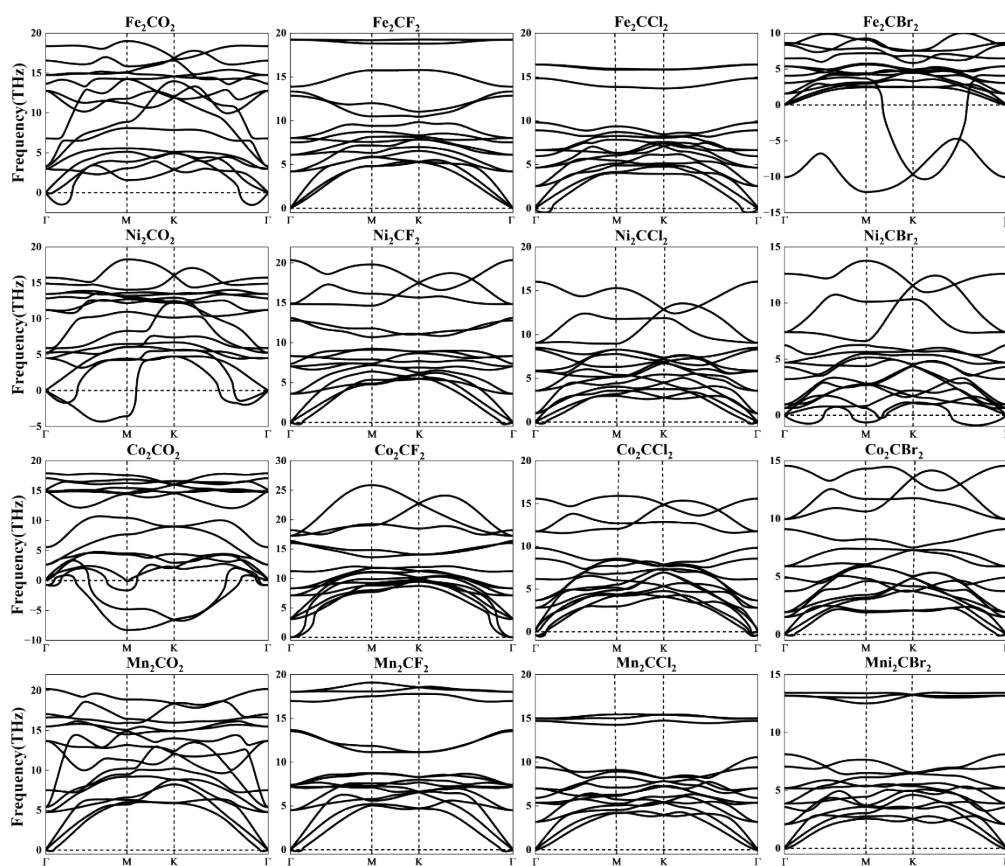


Figure S1 The phonon spectrums of proposed MXenes.

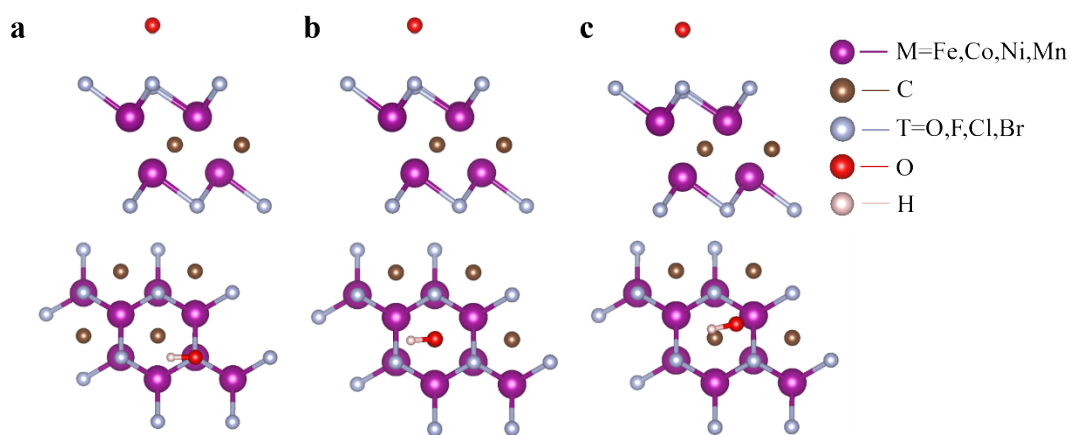


Figure S2. Schematic diagram of OH· adsorption: a-Top b-Hollow c-Bridge.

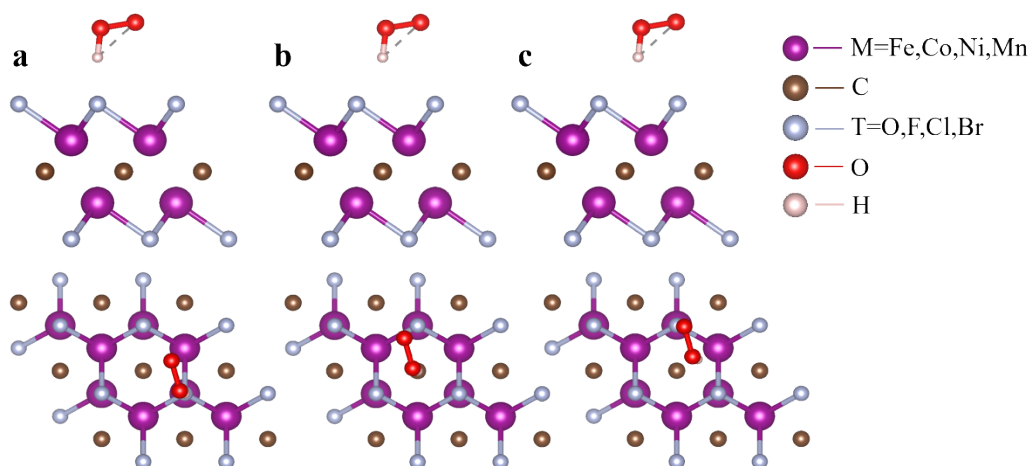


Figure S3 Schematic diagram of HO₂· adsorption: a-Top b-Hollow c-Bridge.

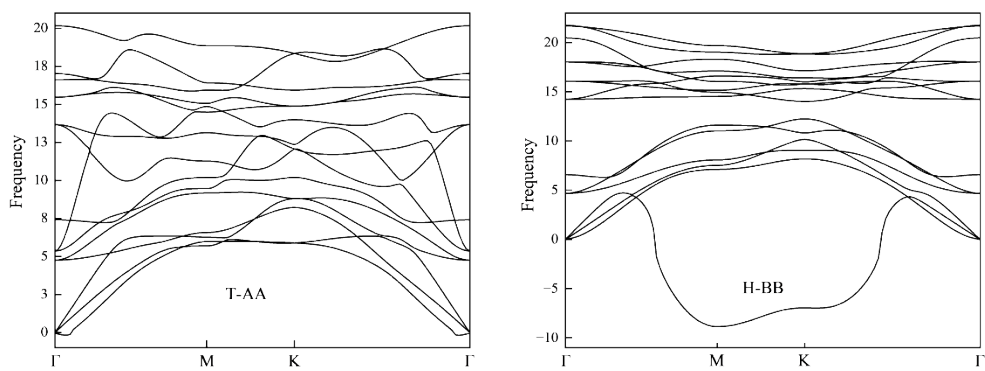


Figure S4 Thermodynamic stability calculation results for different configurations of Mn_2CO_2 .

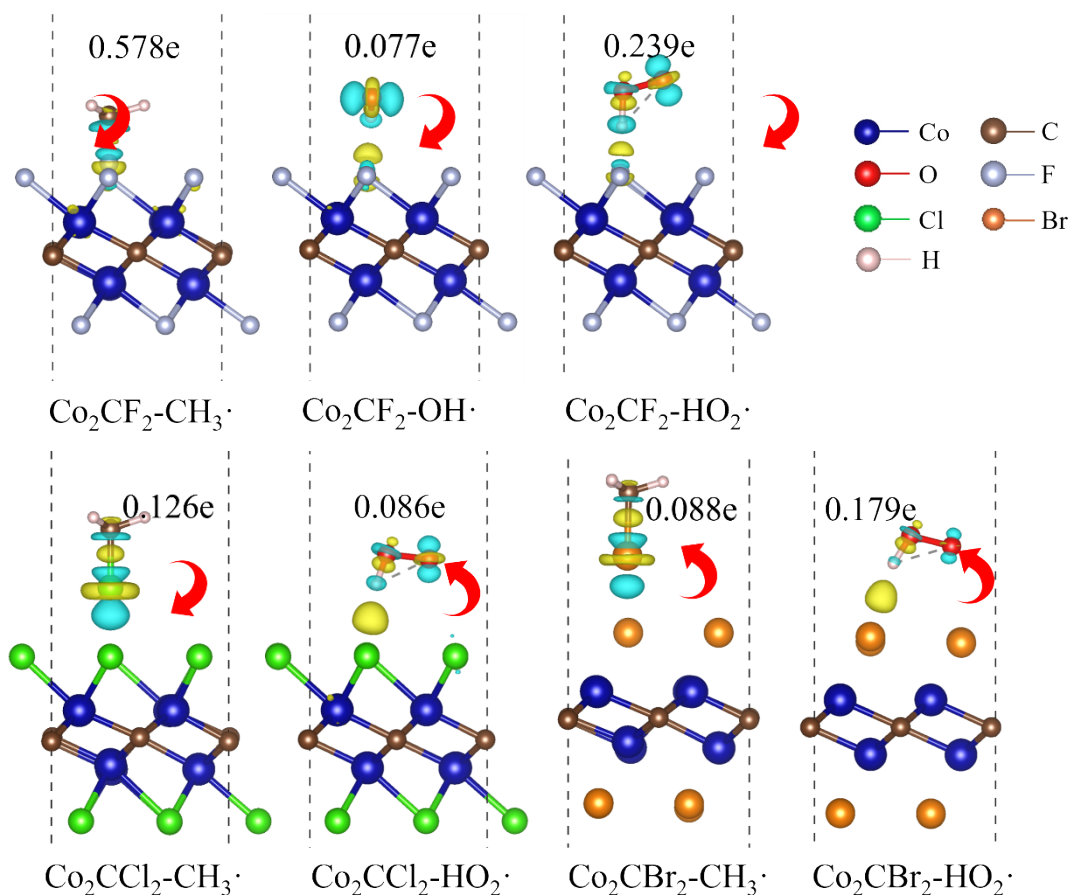


Figure S5 The charge density difference of Co-based MXenes.

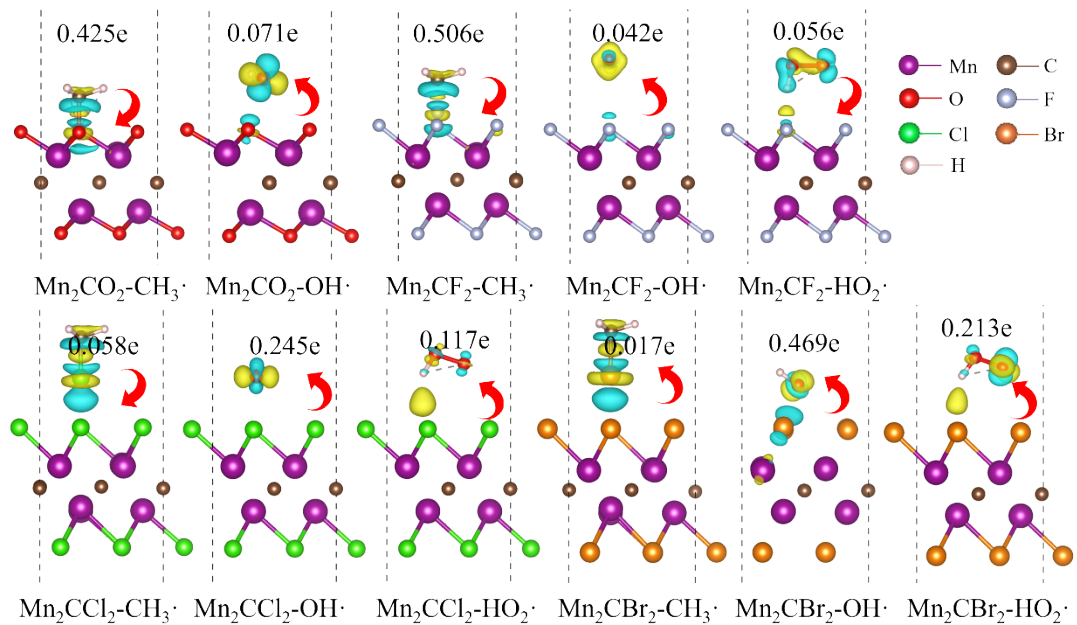


Figure S6 The charge density difference of Mn-based MXenes.

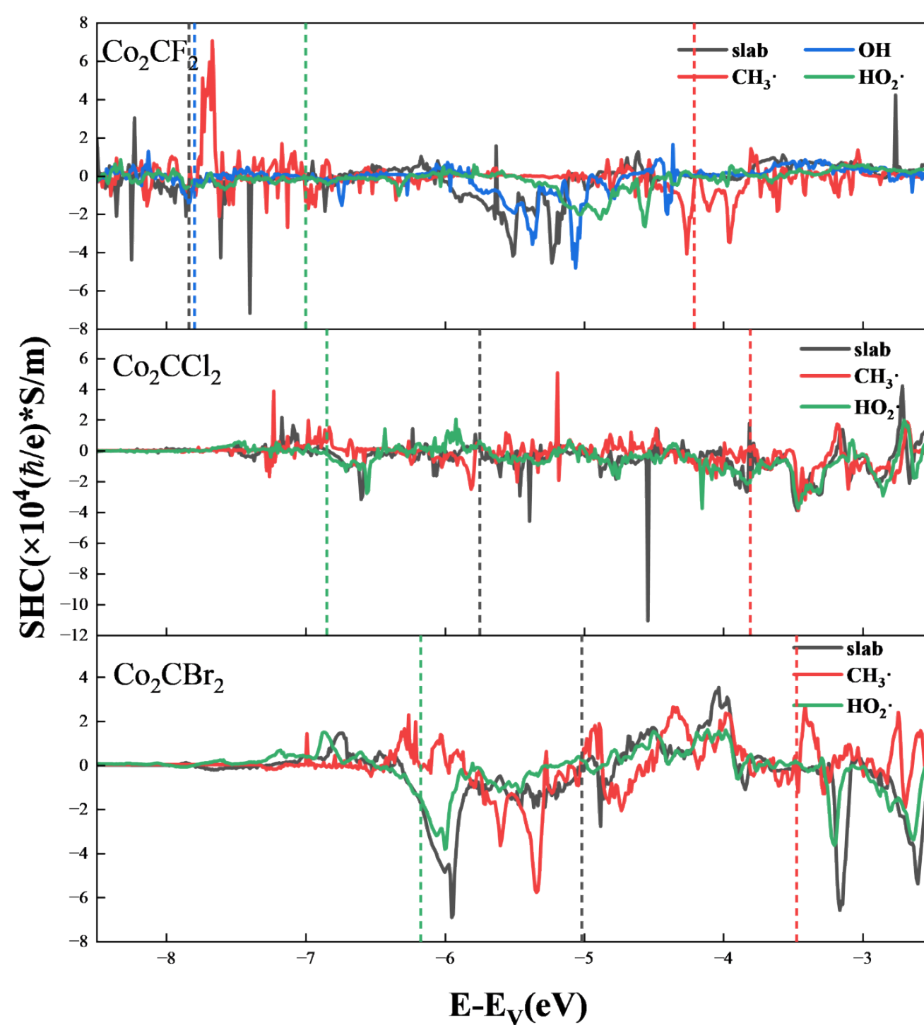


Figure S7 Variation of the SHC of Co-based MXenes as a function of energy ($E - E_v$), with the vacuum level set to 0 eV.

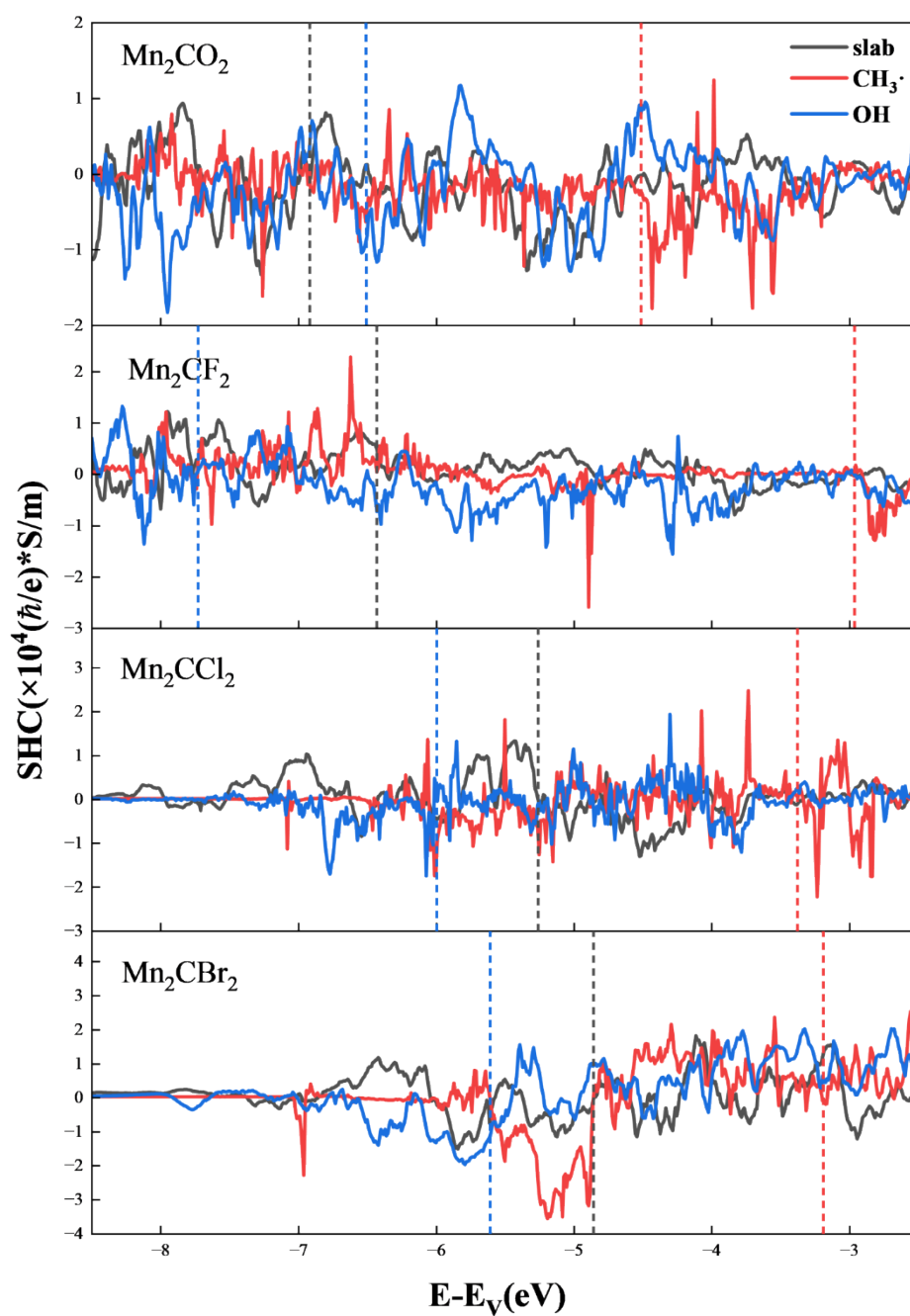


Figure S8 Variation of the SHC of Mn-based MXenes as a function of energy ($E - E_V$), with the vacuum level set to 0 eV.