Supplementary Information

Prediction of Two-Dimensional Metal Ferroelectric Mxenes

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Total Energy Comparison:

Table S1: The total energy comparison of 72 Mxene compositions $(M_2XS_2:M = Sc, Y, Ti, Zr, Hf, V, Nb, Ta, Cr, Mo, W, Mn; X=C, N; S=O, OH, F)$ considering six different crystal structures. Units are in eV and lowest energy for each material is highlighted.

	Sc ₂ NO ₂	Sc₂N(OH)2	Sc ₂ NF ₂	Sc ₂ CO ₂	Sc ₂ C(OH) ₂	Sc ₂ CF ₂
T1	-43.0951	-51.2137	-39.5393	-40.9785	-49.5873	-38.1063
T2	-42.3261	-50.6858	-38.7921	-41.4542	-48.8287	-36.9072
Т3	-42.7873	-50.9465	-39.2009	-41.5231	-49.2217	-37.5281
H1	-42.0521	-49.7851	-37.8741	-40.9023	-48.0079	-37.2890
H2	-42.8936	-50.2739	-38.6330	-40.9802	-48.6882	-37.2890
H3	-42.4343	-50.0277	-38.3246	-40.9539	-48.2194	-36.6561
	Y ₂ NO ₂	Y ₂ N(OH) ₂	Y ₂ NF ₂	Y ₂ CO ₂	Y ₂ C(OH) ₂	Y ₂ CF ₂
T1	-43.3285	-51.0748	-39.4479	-41.253	-49.5798	-38.2083
T2	-42.6755	-50.6796	-38.8867	-41.5365	-48.9700	-37.1773
Т3	-43.1039	-49.2822	-39.2125	-41.6780	-49.2822	-37.7095
H1	-42.3698	-49.6715	-37.8423	-40.9391	-48.0867	-36.3443
H2	-43.0714	-49.9795	-38.2860	-41.1072	-48.5934	-37.2665
H3	-42.6913	-49.8725	-38.1992	-40.9343	-48.3395	-36.8130
	Ti ₂ NO ₂	Ti₂N(OH)₂	Ti ₂ NF ₂	Ti ₂ CO ₂	Ti₂C(OH)₂	Ti ₂ CF ₂
T1	-46.1314	-52.5683	-40.455	-45.1548	-51.8955	-39.8582
Т2	-44.9983	-52.3307	-40.1283	-43.4224	-51.5794	-39.3441
Т3	-45.6145	-52.3037	-40.0638	-44.3901	-51.7727	-39.6547
H1	-44.7456	-51.9311	-39.8397	-43.1824	-50.5473	-38.3494
H2	-45.8115	-51.7139	-39.4368	-44.8272	-50.8379	-38.8717
H3	-45.3421	-51.8048	-39.6800	-44.0464	-50.6971	-38.6023
	Zr ₂ NO ₂	Zr ₂ N(OH) ₂	Zr ₂ NF ₂	Zr ₂ CO ₂	Zr ₂ C(OH) ₂	Zr ₂ CF ₂
T1	-48.7624	-54.1632	-42.0631	-48.0138	-53.8084	-41.8419
T2	-47.6135	-54.1134	-41.9213	-46.0116	-53.6688	-41.5227

Т3	-48.3146	-54.0021	-41.7381	-47.1171	-53.8044	-41.7796
H1	-47.0340	-53.4752	-41.3900	-45.515	-52.2695	-40.1473
H2	-48.1319	-53.1326	-41.0148	-47.3668	-52.3484	-40.3630
H3	-47.7083	-53.2552	-41.1332	-46.4909	-52.3404	-40.2586
	Hf ₂ NO ₂	Hf ₂ N(OH) ₂	Hf_2NF_2	Hf ₂ CO ₂	Hf ₂ C(OH) ₂	Hf ₂ CF ₂
T1	-51.9979	-56.7472	-44.3762	-51.421	-56.6776	-44.5456
T2	-50.8393	-56.8223	-44.5246	-49.2563	-56.5368	-44.2475
Т3	-51.5386	-56.6484	-44.1907	-50.4362	-56.6804	-44.5156
H1	-50.1439	-56.1489	-44.0174	-48.7041	-54.9773	-42.8084
H2	-51.3397	-55.7319	-43.4666	-50.7793	-55.1395	-42.9764
H3	-50.8832	-55.9012	-43.6793	-49.7816	-55.1066	-42.9133
	V ₂ NO ₂	V₂N(OH)₂	V_2NF_2	V ₂ CO ₂	V₂C(OH)₂	V ₂ CF ₂
T1	-45.1796	-52.0141	-39.8067	-44.9353	-51.9408	-39.6926
T2	-45.2036	-51.9769	-39.4984	-44.3574	-51.7800	-39.4295
Т3	-45.1653	-51.7589	-39.3848	-44.6882	-51.6068	-39.2286
H1	-45.3417	-52.1965	-39.7241	-44.1755	-51.8062	-39.5806
H2	-45.2082	-51.9406	-39.7030	-44.6052	-51.3645	-39.0956
H3	-45.1929	-52.1065	-39.7595	-44.4219	-51.5418	-39.2740
	Nb ₂ NO ₂	Nb ₂ N(OH) ₂	Nb ₂ NF ₂	Nb ₂ CO ₂	Nb ₂ C(OH) ₂	Nb ₂ CF ₂
T1	-47.7669	-53.4635	-41.5433	-47.8641	-54.0795	-41.9134
T2	-47.8751	-53.8260	-41.2858	-47.3626	-54.1242	-41.7734
Т3	-47.4946	-53.7121	-40.9264	-47.7048	-53.7153	-41.5013
H1	-47.8375	-53.9650	-41.4398	-46.7022	-53.9721	-41.8226
H2	-47.3105	-53.7679	-41.5341	-47.1109	-53.3820	-41.1665
H3	-47.4915	-53.9772	-41.5959	-46.9300	-53.6435	-41.4243
	1			1		
	Ta ₂ NO ₂	Ta₂N(OH)₂	Ta ₂ NF ₂	Ta ₂ CO ₂	Ta₂C(OH)₂	Ta ₂ CF ₂
T1	-51.9061	-56.6215	-51.9516	-52.2268	-57.5873	-45.1809
T2	-52.1160	-57.3294	-52.1212	-51.6938	-57.7371	-45.1831
T3	-51.6707	-57.1648	-51 6670	E2 0712	-57 2737	-44 7570
114		0712010	-31.0070	-52.0712	57.2757	11.7570
H1	-52.1368	-57.5776	-52.1500	-50.9602	-57.7436	-45.4843
H1 H2	-52.1368 -51.3584	-57.2074	-51.3584	-52.0712 -50.9602 -51.4748	-57.0140	-45.4843 -44.5874
H1 H2 H3	-52.1368 -51.3584 -51.7395	-57.5074 -57.5063	-51.3584 -51.7395	-50.9602 -51.4748 -51.2238	-57.0140 -57.3454	-45.4843 -44.5874 -44.9455
H1 H2 H3	-52.1368 -51.3584 -51.7395	-57.5074 -57.5063	-51.3584 -51.7395	-52.0712 -50.9602 -51.4748 -51.2238	-57.0140 -57.3454	-44.5874 -44.9455
H1 H2 H3	-52.1368 -51.3584 -51.7395 Cr ₂ NO ₂	-57.5776 -57.2074 -57.5063 Cr ₂ N(OH) ₂	-51.3584 -51.7395 Cr ₂ NF ₂	-52.0712 -50.9602 -51.4748 -51.2238 Cr ₂ CO ₂	-57.7436 -57.0140 -57.3454 Cr ₂ C(OH) ₂	-45.4843 -44.5874 -44.9455 Cr ₂ CF ₂
H1 H2 H3 T1	-52.1368 -51.3584 -51.7395 Cr ₂ NO ₂ -43.0892	-57.5776 -57.2074 -57.5063 Cr ₂ N(OH) ₂ -50.4827	-51.0070 -52.1500 -51.3584 -51.7395 Cr ₂ NF ₂ -38.4405	-52.0712 -50.9602 -51.4748 -51.2238 Cr ₂ CO ₂ -43.0775	-57.7436 -57.0140 -57.3454 Cr ₂ C(OH) ₂ -50.2019	-45.4843 -44.5874 -44.9455 Cr ₂ CF ₂ -38.0244
H1 H2 H3 T1 T2	-52.1368 -51.3584 -51.7395 Cr ₂ NO ₂ -43.0892 -43.3605	-57.5776 -57.2074 -57.5063 Cr₂N(OH)₂ -50.4827 -49.6199	-51.0070 -52.1500 -51.3584 -51.7395 Cr ₂ NF ₂ -38.4405 -37.3715	-52.0712 -50.9602 -51.4748 -51.2238 Cr ₂ CO ₂ -43.0775 -43.3605	-57.7436 -57.0140 -57.3454 Cr ₂ C(OH) ₂ -50.2019 -49.7715	-45.4843 -44.5874 -44.9455 Cr ₂ CF ₂ -38.0244 -37.4378
H1 H2 H3 T1 T2 T3	-52.1368 -51.3584 -51.7395 Cr ₂ NO ₂ -43.0892 -43.3605 -43.0281	-57.5776 -57.2074 -57.5063 Cr₂N(OH)₂ -50.4827 -49.6199 -50.1064	-51.0070 -52.1500 -51.3584 -51.7395 Cr₂NF₂ -38.4405 -37.3715 -37.9166	-52.0712 -50.9602 -51.4748 -51.2238 Cr₂CO₂ -43.0775 -43.3605 -43.1826	-57.7436 -57.0140 -57.3454 Cr₂C(OH)₂ -50.2019 -49.7715 -50.0825	-45.4843 -44.5874 -44.9455 Cr ₂ CF ₂ -38.0244 -37.4378 -37.8134
H1 H2 H3 T1 T2 T3 H1	-52.1368 -51.3584 -51.7395 Cr ₂ NO ₂ -43.0892 -43.3605 -43.0281 -43.7804	-57.5776 -57.2074 -57.5063 Cr₂N(OH)₂ -50.4827 -49.6199 -50.1064 -49.8074	-51.0070 -52.1500 -51.3584 -51.7395 Cr ₂ NF ₂ -38.4405 -37.3715 -37.9166 -37.5663	-52.0712 -50.9602 -51.4748 -51.2238 Cr₂CO₂ -43.0775 -43.3605 -43.1826 -43.7656	-57.7436 -57.0140 -57.3454 Cr ₂ C(OH) ₂ -50.2019 -49.7715 -50.0825 -50.0087	-45.4843 -44.5874 -44.9455 Cr ₂ CF ₂ -38.0244 -37.4378 -37.8134 -37.6990
H1 H2 H3 T1 T2 T3 H1 H2	-52.1368 -51.3584 -51.7395 Cr ₂ NO ₂ -43.0892 -43.3605 -43.0281 -43.7804 -43.3197	-57.5776 -57.2074 -57.5063 Cr₂N(OH)₂ -50.4827 -49.6199 -50.1064 -49.8074 -50.2246	-51.0070 -52.1500 -51.3584 -51.7395 Cr₂NF₂ -38.4405 -37.3715 -37.9166 -37.5663 -37.9861	-52.0712 -50.9602 -51.4748 -51.2238 Cr₂CO₂ -43.0775 -43.3605 -43.1826 -43.7656 -43.3197	-57.7436 -57.0140 -57.3454 Cr ₂ C(OH) ₂ -50.2019 -49.7715 -50.0825 -50.0087 -50.0626	-45.4843 -44.5874 -44.9455 Cr ₂ CF ₂ -38.0244 -37.4378 -37.8134 -37.6990 -37.8919
H1 H2 H3 T1 T2 T3 H1 H2 H3	-52.1368 -51.3584 -51.7395 Cr2NO2 -43.0892 -43.3605 -43.0281 -43.7804 -43.3197 -43.4670	-57.5776 -57.2074 -57.5063 Cr ₂ N(OH) ₂ -50.4827 -49.6199 -50.1064 -49.8074 -50.2246 -49.9732	-51.0070 -52.1500 -51.3584 -51.7395 Cr ₂ NF ₂ -38.4405 -37.3715 -37.9166 -37.5663 -37.9861 -37.7080	-52.0712 -50.9602 -51.4748 -51.2238 Cr ₂ CO ₂ -43.0775 -43.3605 -43.1826 -43.7656 -43.3197 -43.4670	-57.7436 -57.0140 -57.3454 Cr ₂ C(OH) ₂ -50.2019 -49.7715 -50.0825 -50.0087 -50.0626 -50.0495	-44.5874 -44.5874 -44.9455 Cr ₂ CF ₂ -38.0244 -37.4378 -37.8134 -37.6990 -37.8919 -37.8092
H1 H2 H3 T1 T2 T3 H1 H2 H3	-52.1368 -51.3584 -51.7395 Cr ₂ NO ₂ -43.0892 -43.3605 -43.0281 -43.7804 -43.3197 -43.4670	-57.5776 -57.2074 -57.5063 Cr₂N(OH)₂ -50.4827 -49.6199 -50.1064 -49.8074 -50.2246 -49.9732	-51.0070 -52.1500 -51.3584 -51.7395 Cr ₂ NF ₂ -38.4405 -37.3715 -37.9166 -37.5663 -37.9861 -37.7080	-52.0712 -50.9602 -51.4748 -51.2238 Cr ₂ CO ₂ -43.0775 -43.3605 -43.1826 -43.7656 -43.3197 -43.4670	-57.7436 -57.0140 -57.3454 Cr₂C(OH)₂ -50.2019 -49.7715 -50.0825 -50.0087 -50.0626 -50.0495	-45.4843 -44.5874 -44.9455 Cr ₂ CF ₂ -38.0244 -37.4378 -37.8134 -37.6990 -37.8919 -37.8092

-45.6724	-52.1984	-39.7759	-45.9179	-52.1834	-40.5013			
-46.7709	-51.6272	-39.2256	-47.1149	-52.7117	-40.2910			
-46.3498	-51.8219	-40.1646	-46.3995	-52.4871	-40.0833			
-47.0909	-52.0129	-39.6644	-47.5423	-52.9049	-40.4838			
-46.5615	-52.7942	-40.5122	-46.5417	-52.9691	-40.7571			
-46.9263	-52.4377	-40.0294	-46.9038	-52.9992	-40.7019			
W ₂ NO ₂	W ₂ N(OH) ₂	W_2NF_2	W ₂ CO ₂	W ₂ C(OH) ₂	W ₂ CF ₂			
-49.9652	-55.4397	-42.8996	-50.1858	-55.5289	-43.6156			
-50.5922	-54.4791	-41.8730	-51.4844	-56.1021	-43.4573			
-50.2895	-55.0175	-42.3181	-50.5953	-55.8540	-43.2184			
-50.9929	-55.1403	-42.4529	-52.1072	-56.5309	-43.9095			
-50.4194	-56.0201	-43.57605	-50.8589	-56.4858	-44.1008			
-50.8756	-55.6462	-43.0438	-51.3038	-56.5941	-44.0844			
Mn ₂ NO ₂	Mn ₂ N(OH) ₂	Mn ₂ NF ₂	Mn ₂ CO ₂	Mn ₂ C(OH) ₂	Mn ₂ CF ₂			
-41.6585	-49.0458	-36.9699	-41.0790	-49.1869	-37.0995			
-40.5312	-47.1151	-36.1395	-40.8113	-48.3219	-36.1066			
-41.2226	-48.3894	-36.2711	-40.6936	-48.7615	-36.6307			
-40.6999	-48.1382	-35.8886	-41.0701	-48.1650	-35.9332			
-41.6864	-48.5865	-36.5857	-40.8092	-48.9296	-36.7994			
-40.9475	-48.5443	-36.4228	-41.0067	-48.5319	-36.3489			
	-45.6724 -46.7709 -46.3498 -47.0909 -46.5615 -46.9263 W2NO2 -49.9652 -50.5922 -50.2895 -50.2895 -50.4194 -50.8756 Mn2NO2 -41.6585 -40.5312 -41.2226 -40.6999 -41.6864 -40.9475	-45.6724 -52.1984 -46.7709 -51.6272 -46.3498 -51.8219 -47.0909 -52.0129 -46.5615 -52.7942 -46.9263 -52.4377 W2NO2 W2N(OH)2 -49.9652 -55.4397 -50.5922 -54.4791 -50.2895 -55.0175 -50.9929 -55.1403 -50.4194 -56.0201 -50.8756 -55.6462 Mn2NO2 Mn2N(OH)2 -41.6585 -49.0458 -40.5312 -47.1151 -41.2226 -48.3894 -40.6999 -48.1382 -41.6864 -48.5865 -40.9475 -48.5443	-45.6724-52.1984-39.7759-46.7709-51.6272-39.2256-46.3498-51.8219-40.1646-47.0909-52.0129-39.6644-46.5615-52.7942-40.5122-46.9263-52.4377-40.0294W2NO2W2N(OH)2W2NF2-49.9652-55.4397-42.8996-50.5922-54.4791-41.8730-50.2895-55.0175-42.3181-50.9929-55.1403-42.4529-50.4194-56.0201-43.57605-50.8756-55.6462-43.0438Mn2NO2Mn2N(OH)2Mn2NO2-47.1151-36.1395-41.6585-49.0458-36.9699-40.5312-47.1151-36.1395-41.2226-48.3894-36.2711-40.6999-48.1382-35.8886-41.6864-48.5865-36.5857-40.9475-48.5443-36.4228	-45.6724 -52.1984 -39.7759 -45.9179 -46.7709 -51.6272 -39.2256 -47.1149 -46.3498 -51.8219 -40.1646 -46.3995 -47.0909 -52.0129 -39.6644 -47.5423 -46.5615 -52.7942 -40.5122 -46.5417 -46.9263 -52.4377 -40.0294 -46.9038 W2NO2 W2N(OH)2 W2NF2 W2CO2 -49.9652 -55.4397 -42.8996 -50.1858 -50.5922 -54.4791 -41.8730 -51.4844 -50.2895 -55.0175 -42.3181 -50.5953 -50.4194 -56.0201 -43.57605 -50.8589 -50.8756 -55.6462 -43.0438 -51.3038 Mn2NO2 Mn2N(OH)2 Mn2NF2 Mn2CO2 -41.6585 -49.0458 -36.9699 -41.0790 -40.5312 -47.1151 -36.1395 -40.8113 -41.2226 -48.3894 -36.2711 -40.6936 -40.6999 -48.1382 -35.8886 -41.0701 -41.6864 -48.5865 -36.5857 -	-45.6724 -52.1984 -39.7759 -45.9179 -52.1834 -46.7709 -51.6272 -39.2256 -47.1149 -52.7117 -46.3498 -51.8219 -40.1646 -46.3995 -52.4871 -47.0909 -52.0129 -39.6644 -47.5423 -52.9049 -46.5615 -52.7942 -40.5122 -46.5417 -52.9691 -46.9263 -52.4377 -40.0294 -46.9038 -52.9992 - - -52.4377 -40.0294 -46.9038 -52.9992 -46.9263 -52.4377 -40.0294 -46.9038 -52.9992 - - - -46.9038 -52.9992 - - - -52.4377 -40.0294 -46.9038 -52.9992 -49.9652 -55.4397 -42.8996 -50.1858 -55.5289 -50.5922 -54.4791 -41.8730 -51.4844 -56.1021 -50.2895 -55.0175 -42.3181 -50.5953 -55.8540 -50.462 -43.0438 -51.3038 -56.5941 -50.8192 -55.6462 -43.0438 -51.3			

Phonon calculations:

Finite displacement method was use to obtain phonon band structures using PHONOPY code²⁷. Supercell of 4×4×1 and K-point mesh of 5×5×1 was used to obtain interatomic forces using VASP code. However, calculations are limited to smaller supercells due to limitations in



computational power.

Figure S1: Calculated phonon band structures of 2D (a) $Nb_2N(OH)_2$ (b) $W_2C(OH)_2$ and (c) $Mo_2C(OH)_2$.

Bader Charge Analysis: -



Figure S2: Excess bader charge on atoms calculated by conducting bader charge analysis.



Graphene/Nb₂NF₂ heterostructure: -

Figure S3: In-plane averaged electrostatic potential for monolayer Nb_2NF_2 and Monolayer Graphene heterostructure with polarization acting (a) downwards and (b) upwards. Here,

fermi level and work function are indicated in E_f and Φ . Polarization direction and out of plane direction(Z(Å)) are indicated by orange and blue coloured arrows, respectively.