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_2NO_2	$Sc_2N(OH)2$	Sc_2NF_2	Sc_2CO_2	$Sc_2C(OH)_2$	Sc_2CF_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
T3	-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_2NO_2	$Y_2N(OH)_2$	Y_2NF_2	Y_2CO_2	$Y_2C(OH)_2$	Y_2CF_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
T3	-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_2NO_2	$Ti_2N(OH)_2$	Ti_2NF_2	Ti_2CO_2	$Ti_2C(OH)_2$	Ti_2CF_2
T1	**-46.1314**	**-52.5683**	**-40.455**	**-45.1548**	**-51.8955**	**-39.8582**
T2	-44.9983	-52.3307	-40.1283	-43.4224	-51.5794	-39.3441
T3	-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_2NO_2	$Zr_2N(OH)_2$	Zr_2NF_2	Zr_2CO_2	$Zr_2C(OH)_2$	Zr_2CF_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

T3	-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_2NO_2	**$Hf_2N(OH)_2$**	**Hf_2NF_2**	**Hf_2CO_2**	**$Hf_2C(OH)_2$**	**Hf_2CF_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
T3	-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_2NO_2	**$V_2N(OH)_2$**	**V_2NF_2**	**V_2CO_2**	**$V_2C(OH)_2$**	**V_2CF_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
T3	-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_2NO_2	**$Nb_2N(OH)_2$**	**Nb_2NF_2**	**Nb_2CO_2**	**$Nb_2C(OH)_2$**	**Nb_2CF_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
T3	-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
	Ta_2NO_2	**$Ta_2N(OH)_2$**	**Ta_2NF_2**	**Ta_2CO_2**	**$Ta_2C(OH)_2$**	**Ta_2CF_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	-52.0712	-57.2737	-44.7570
H1	**-52.1368**	**-57.5776**	**-52.1500**	-50.9602	**-57.7436**	**-45.4843**
H2	-51.3584	-57.2074	-51.3584	-51.4748	-57.0140	-44.5874
H3	-51.7395	-57.5063	-51.7395	-51.2238	-57.3454	-44.9455
	Cr_2NO_2	**$Cr_2N(OH)_2$**	**Cr_2NF_2**	**Cr_2CO_2**	**$Cr_2C(OH)_2$**	**Cr_2CF_2**
T1	-43.0892	**-50.4827**	**-38.4405**	-43.0775	**-50.2019**	**-38.0244**
T2	-43.3605	-49.6199	-37.3715	-43.3605	-49.7715	-37.4378
T3	-43.0281	-50.1064	-37.9166	-43.1826	-50.0825	-37.8134
H1	**-43.7804**	-49.8074	-37.5663	**-43.7656**	-50.0087	-37.6990
H2	-43.3197	-50.2246	-37.9861	-43.3197	-50.0626	-37.8919
H3	-43.4670	-49.9732	-37.7080	-43.4670	-50.0495	-37.8092
	Mo_2NO_2	**$Mo_2N(OH)_2$**	**Mo_2NF_2**	**Mo_2CO_2**	**$Mo_2C(OH)_2$**	**Mo_2CF_2**

T1	-45.6724	-52.1984	-39.7759	-45.9179	-52.1834	-40.5013
T2	-46.7709	-51.6272	-39.2256	-47.1149	-52.7117	-40.2910
T3	-46.3498	-51.8219	-40.1646	-46.3995	-52.4871	-40.0833
H1	**-47.0909**	-52.0129	-39.6644	**-47.5423**	-52.9049	-40.4838
H2	-46.5615	**-52.7942**	**-40.5122**	-46.5417	-52.9691	**-40.7571**
H3	-46.9263	-52.4377	-40.0294	-46.9038	**-52.9992**	-40.7019
	W_2NO_2	**$W_2N(OH)_2$**	**W_2NF_2**	**W_2CO_2**	**$W_2C(OH)_2$**	**W_2CF_2**
T1	-49.9652	-55.4397	-42.8996	-50.1858	-55.5289	-43.6156
T2	-50.5922	-54.4791	-41.8730	-51.4844	-56.1021	-43.4573
T3	-50.2895	-55.0175	-42.3181	-50.5953	-55.8540	-43.2184
H1	**-50.9929**	-55.1403	-42.4529	**-52.1072**	-56.5309	-43.9095
H2	-50.4194	**-56.0201**	**-43.57605**	-50.8589	-56.4858	**-44.1008**
H3	-50.8756	-55.6462	-43.0438	-51.3038	**-56.5941**	-44.0844
	Mn_2NO_2	**$Mn_2N(OH)_2$**	**Mn_2NF_2**	**Mn_2CO_2**	**$Mn_2C(OH)_2$**	**Mn_2CF_2**
T1	-41.6585	**-49.0458**	**-36.9699**	**-41.0790**	**-49.1869**	**-37.0995**
T2	-40.5312	-47.1151	-36.1395	-40.8113	-48.3219	-36.1066
T3	-41.2226	-48.3894	-36.2711	-40.6936	-48.7615	-36.6307
H1	-40.6999	-48.1382	-35.8886	-41.0701	-48.1650	-35.9332
H2	**-41.6864**	-48.5865	-36.5857	-40.8092	-48.9296	-36.7994
H3	-40.9475	-48.5443	-36.4228	-41.0067	-48.5319	-36.3489

Phonon calculations:

Finite displacement method was use to obtain phonon band structures using PHONOPY code[27]. 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.

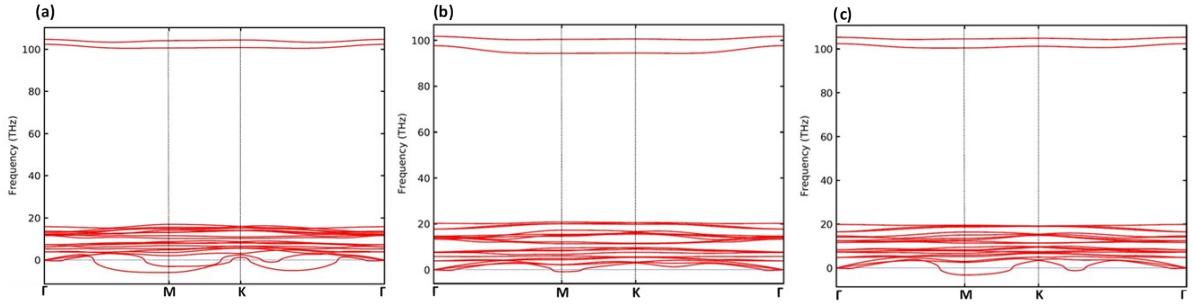

Figure S1: Calculated phonon band structures of 2D (a) $Nb_2N(OH)_2$ (b) $W_2C(OH)_2$ and (c) $Mo_2C(OH)_2$.

Bader Charge Analysis: -

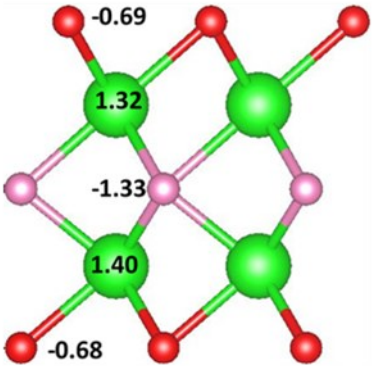

Figure S2: Excess bader charge on atoms calculated by conducting bader charge analysis.

Graphene/Nb_2NF_2 heterostructure: -

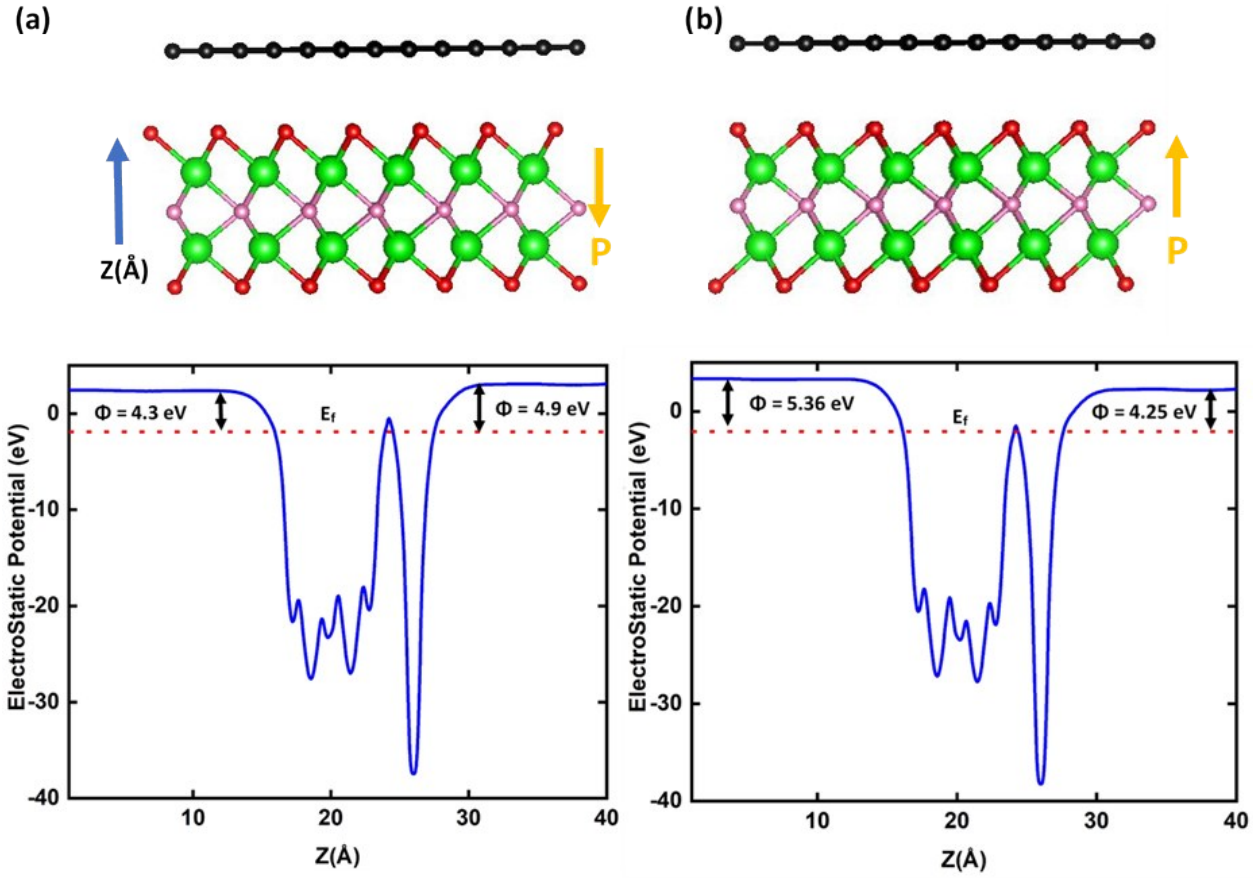

Figure S3: In-plane averaged electrostatic potential for monolayer Nb_2NF_2 and Monolayer Graphene heterostructure with polarization acting (a) downwards and (b) upwards. Here,

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.