Electronic Supplementary Material (ESI) for RSC Advances.

Ti_3BN monolayer: the MXene-like material predicted by first-principles calculations

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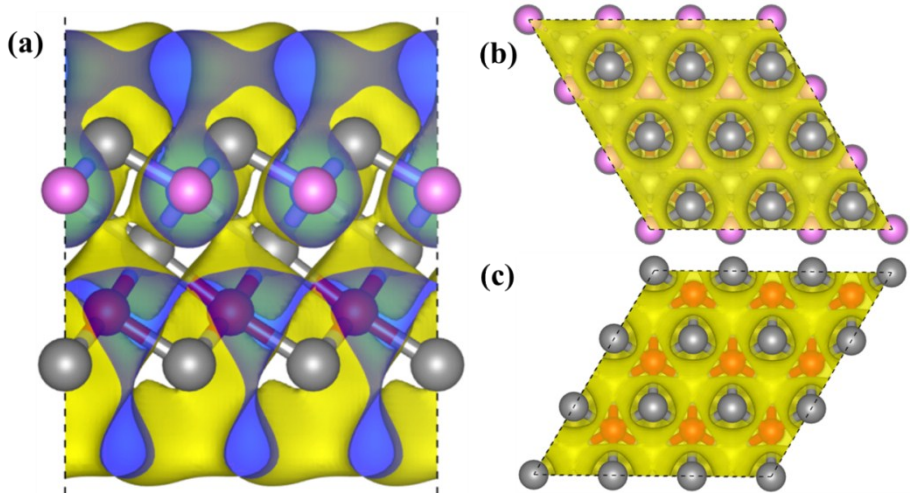

Figure S1. (a) Side view, (b) top view, and (c) bottom view of isosurface of electron localization function plotted with the value of 0.3 au. The yellow regions denote the electron accumulation. Gray, pink and red balls represent Ti, N and B atoms, respectively.

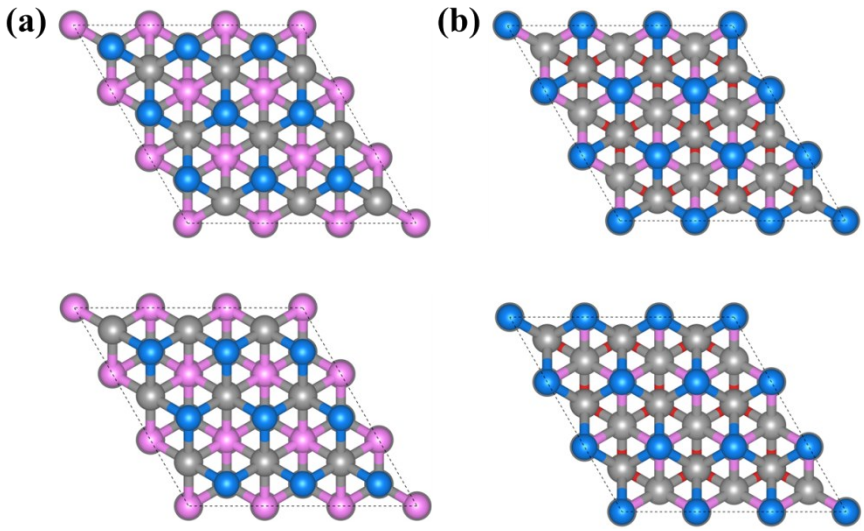

Figure S2. Top (upper) and bottom (lower) views of (a) Ti_3BNF_2-I, (b) Ti_3BNF_2-II. Gray, pink and red balls represent Ti, N and B atoms, respectively. The F atoms are indicated by cyan balls.

Table **S1**. Lattice constants, bond lengths and band gaps of Ti_3BN monolayer with bare, hydroxylated, and fluorinated surfaces.

Geometry configuration	Lattice constants, a,b (Å)	Bond length (Å)						Band gap (eV)
		T-Ti_1	Ti_1-N	N-Ti_2	Ti_2-B	B-Ti_3	Ti_3-T_2	
$Ti_3BN(OH)_2$-I	3.080	2.183	2.067	2.177	2.223	2.152	2.180	0
$Ti_3BN(OH)_2$-II	3.031	2.175	2.103	2.150	2.208	2.164	2.190	0.160 (direct)
$Ti_3BN(OH)_2$-III	3.066	2.175	2.067	2.174	2.212	2.168	2.205	0
$Ti_3BN(OH)_2$-IV	3.045	2.181	2.107	2.153	2.213	2.147	2.165	0.090 (direct)
Ti_3BN	3.095	--	2.054	2.195	2.249	2.117	--	0
Ti_3BNF_2-I	3.058	2.168	2.050	2.172	2.219	2.143	2.151	0
Ti_3BNF_2-II	2.989	2.158	2.093	2.134	2.197	2.152	2.172	0.070 (indirect)
Ti_3BNF_2-III	3.042	2.160	2.048	2.171	2.200	2.161	2.194	0
Ti_3BNF_2-IV	3.008	2.167	2.101	2.136	2.209	2.134	2.134	0.370 (indirect)