Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

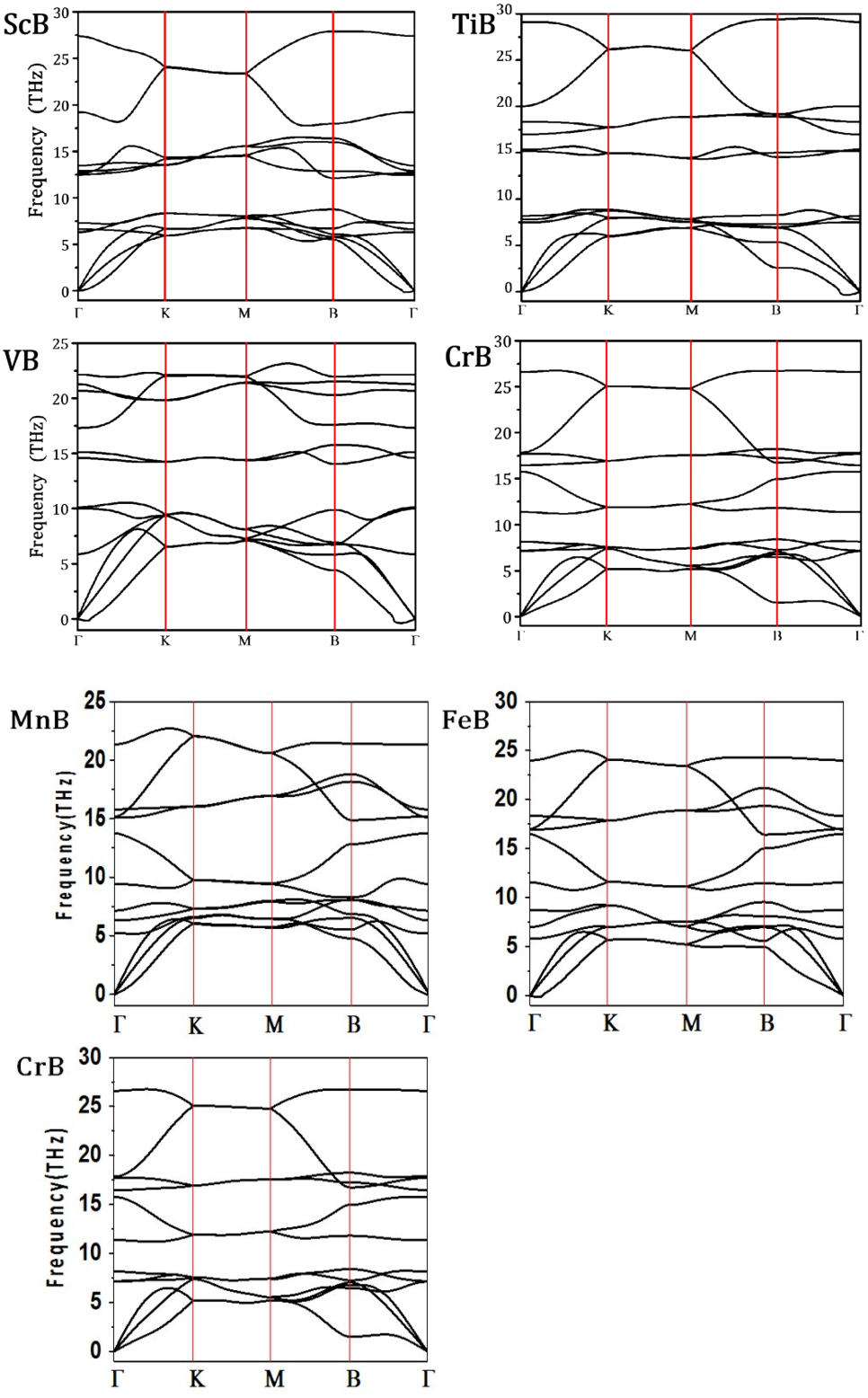
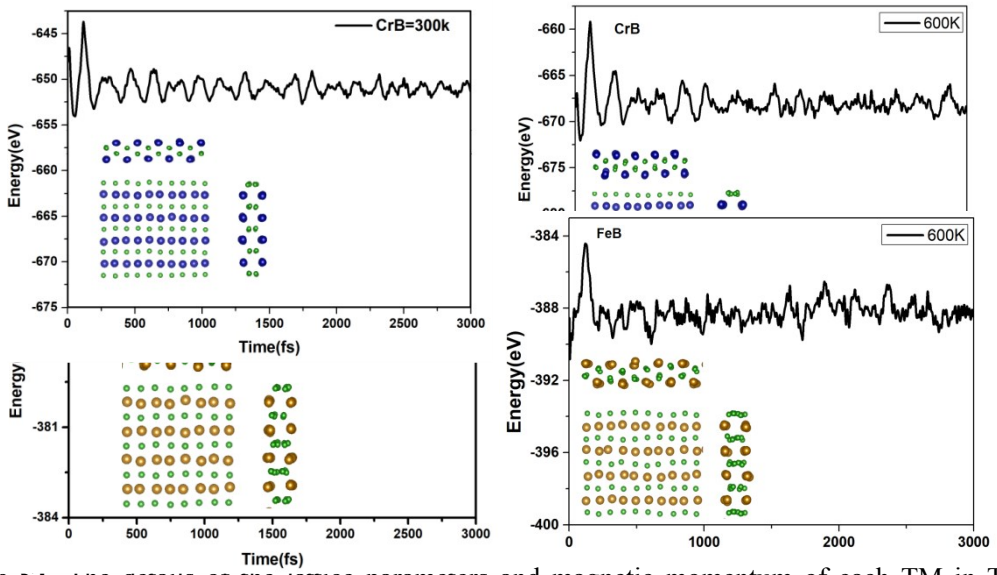




**Figure S1.** Calculated phonon band structures for TMB (TM=TM=Co, Cr, Fe, Mn, Sc, Ti,) monolayer. Similar to phonon spectra of the Ge monolayer[1] and borophene[2], the tiny imaginary frequency nearing the Γ point is also found, although the Ge monolayer and borophene have been experimentally realized on the surface of metal substrate.[2-7]



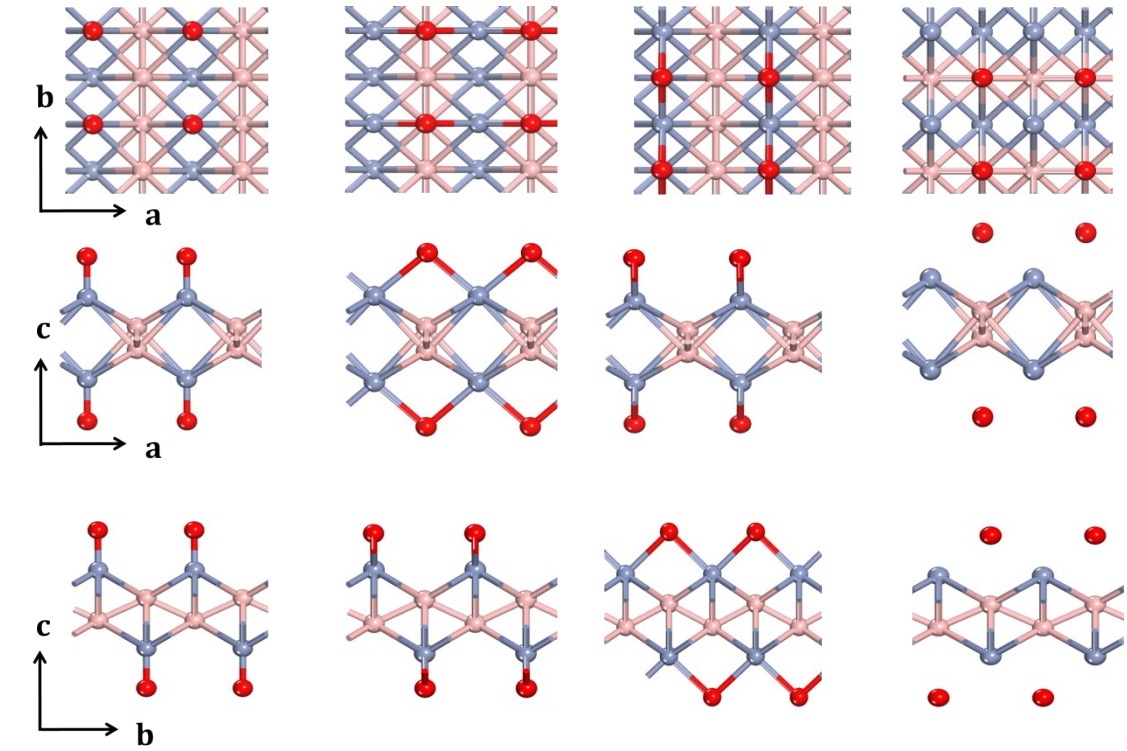

**Fi** 300 K

**Table S1**. The details of the lattice parameters and magnetic momentum of each TM in TMB (TM=Co, Cr, Fe, Mn, Sc, Ti) monolayers. The results are obtained with GGA+U calculation.

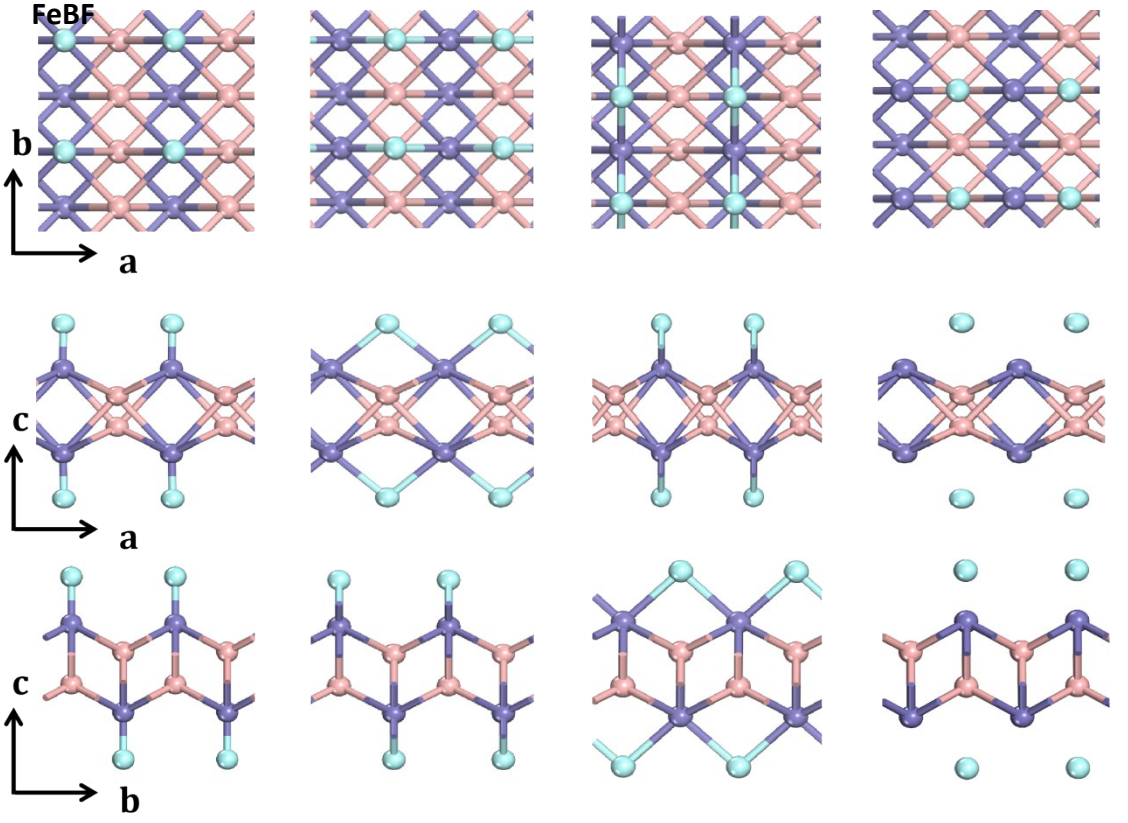
| 2D monolayer | a( Å) | b( Å) | $M_{TM}$ $(\mu_B)$ |
|---|---|---|---|
| **CoB** | 2.59 | 2.90 | 0.48 |
| **CrB** | 2.93 | 2.87 | 3.50 |
| **FeB** | 2.77 | 2.82 | 2.70 |
| **MnB** | 2.90 | 2.87 | 3.70 |
| **ScB** | 3.30 | 3.09 | 0.09 |
| **TiB** | 3.10 | 2.96 | 0.53 |
| **VB** | 3.18 | 2.91 | 0.004 |

**CrBO**

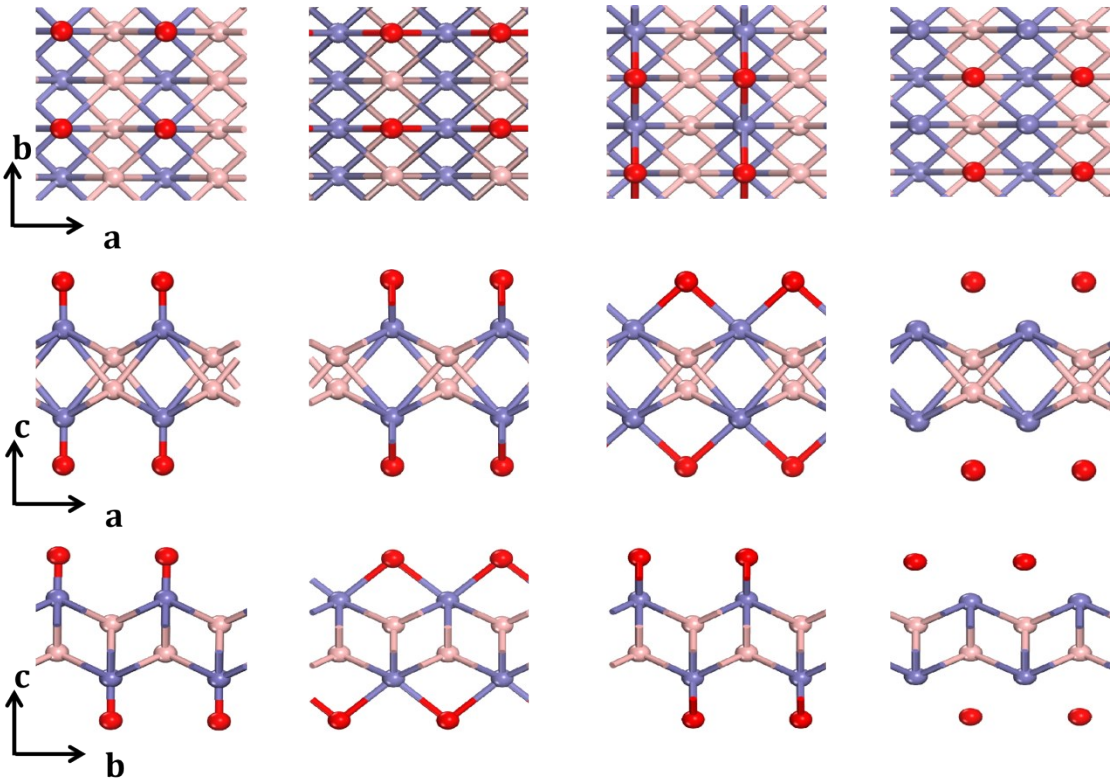
**P1** **P2** **P3** **P4**



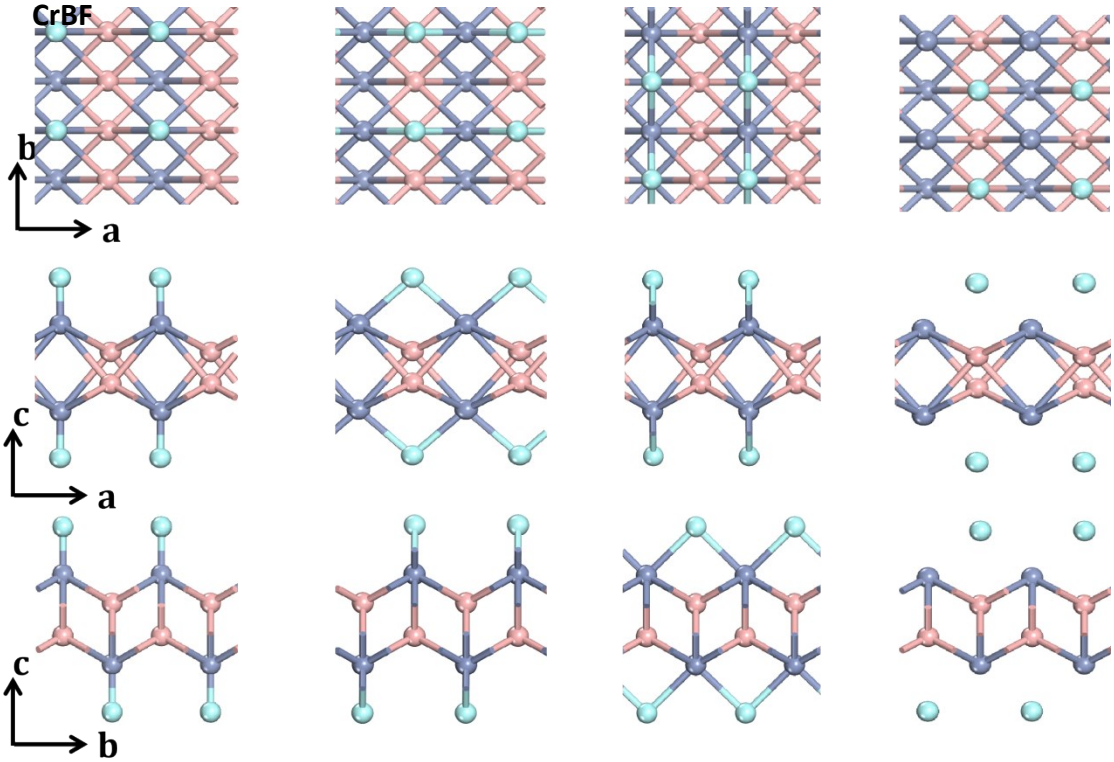

FeBF




FeBO




CrBF




FeBOH

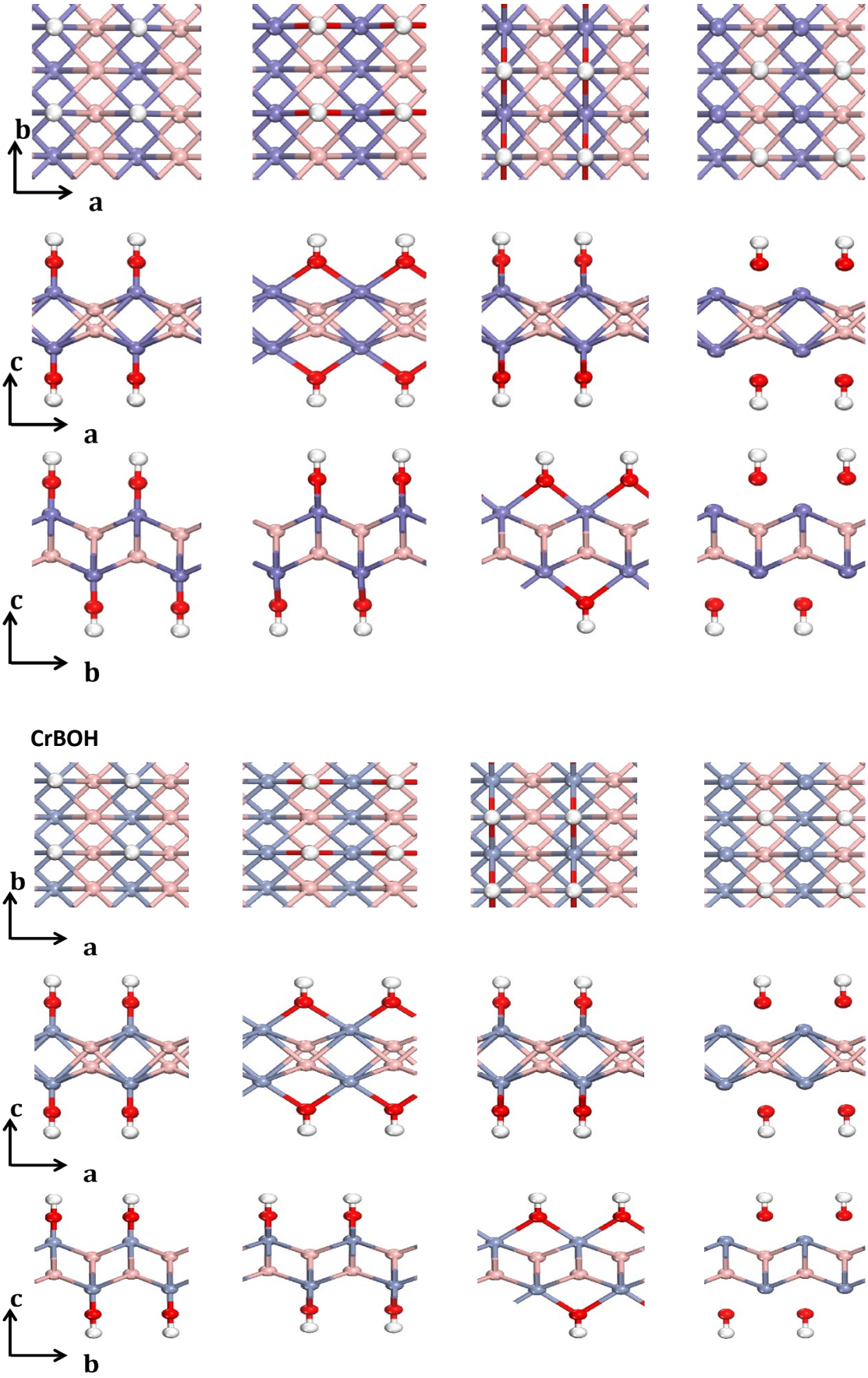



**Figure S3.** In this work, we considered four possible positions (P1, P2, P3 and P4) for F, O and OH functional groups adsorbing on the 2D TMB monolayer as shown in Figure S2.

**Table S2.** The adsorption energies ($E_f$) of the TMBX(X=F,O,OH) monolayer in four forms respectively. The adsorption energies is described as: $E_f = \left(E_{TMBX} - E_{TMB} - nE_X\right)/n$

| $E_f$(eV) | CrBF | CrBOH | CrBO | FeBO | FeBF | FeBOH |
|---|---|---|---|---|---|---|
| **P1** | -4.61 | -3.85 | -4.65 | -3.54 | -3.64 | -3.68 |
| **P2** | -4.41 | -3.87 | -4.95 | -3.74 | -3.65 | -3.70 |
| **P3** | -4.69 | -4.20 | -5.28 | -3.66 | -3.64 | -3.63 |
| **P4** | -3.62 | -3.22 | -4.42 | -3.37 | -2.96 | -3.23 |

**Table S3.** The total energies of the unit cell of TMBX(X=F,O,OH) in four forms respectively.

| Total Energy(eV) | CrBF | CrBOH | CrBO | FeBO | FeBF | FeBOH |
|---|---|---|---|---|---|---|
| **P1** | -43.08 | -54.44 | -39.60 | -32.32 | -39.11 | -52.01 |
| **P2** | -42.67 | -54.48 | -40.16 | -32.56 | -39.12 | -52.04 |
| **P3** | -43.24 | -55.12 | -40.80 | -32.55 | -39.11 | -51.90 |
| **P4** | -41.09 | -53.13 | -39.10 | -31.97 | -37.75 | -51.10 |

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