

Fig. S1 Side views of the optimized lattice structures of (a) I- $\text{Ti}_3\text{N}_2\text{F}_2$, (b) II- $\text{Ti}_3\text{N}_2\text{F}_2$, (c) III- $\text{Ti}_3\text{N}_2\text{F}_2$, (d) I- $\text{Ti}_3\text{N}_2\text{O}_2$, (e) II- $\text{Ti}_3\text{N}_2\text{O}_2$, (f) III- $\text{Ti}_3\text{N}_2\text{O}_2$, (g) I- $\text{Ti}_3\text{N}_2(\text{OH})_2$, (h) II- $\text{Ti}_3\text{N}_2(\text{OH})_2$, (i) III- $\text{Ti}_3\text{N}_2(\text{OH})_2$. Top views of (j) I- $\text{Ti}_3\text{N}_2\text{F}_2$, (k) II- $\text{Ti}_3\text{N}_2\text{F}_2$ monolayers.

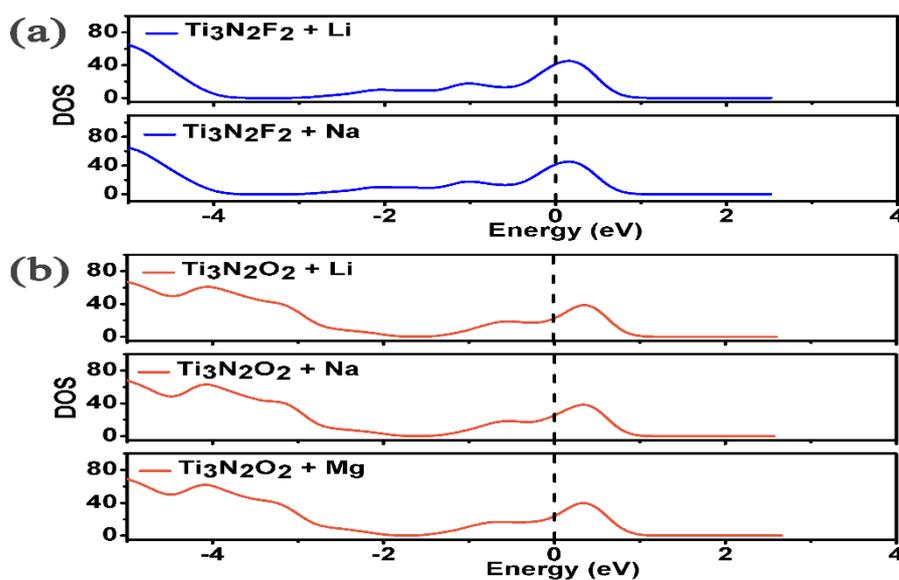


Fig. S2 Total DOS of the (a) the $\text{Ti}_3\text{N}_2\text{F}_2$ monolayer after Li and Na adsorption, (b) the $\text{Ti}_3\text{N}_2\text{O}_2$ monolayer after Li, Na and Mg adsorption. The Fermi levels are set to zero and are indicated by the dashed lines.