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Investigation of Chloride Ion Adsorption onto Ti_2C MXene Monolayers by First-principles Calculations

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Supporting Information

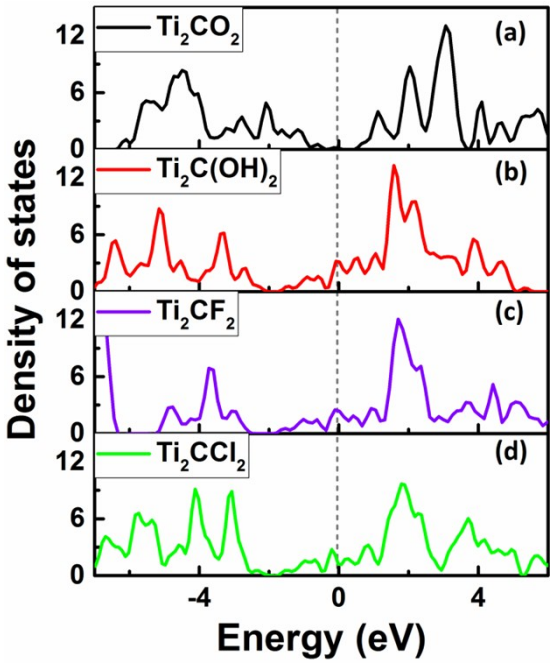

Fig. S1. Density of states (DOS) of (a) Ti_2CO_2, (b) $Ti_2C(OH)_2$, (c) Ti_2CF_2, and (d) Ti_2CCl_2 monolayers, respectively.

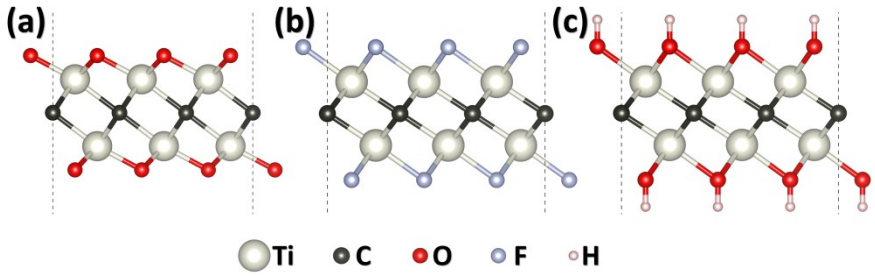

Fig. S2. Side views of (a) Ti_2CO_2, (b) Ti_2CF_2, and (a) $Ti_2C(OH)_2$ monolayers.

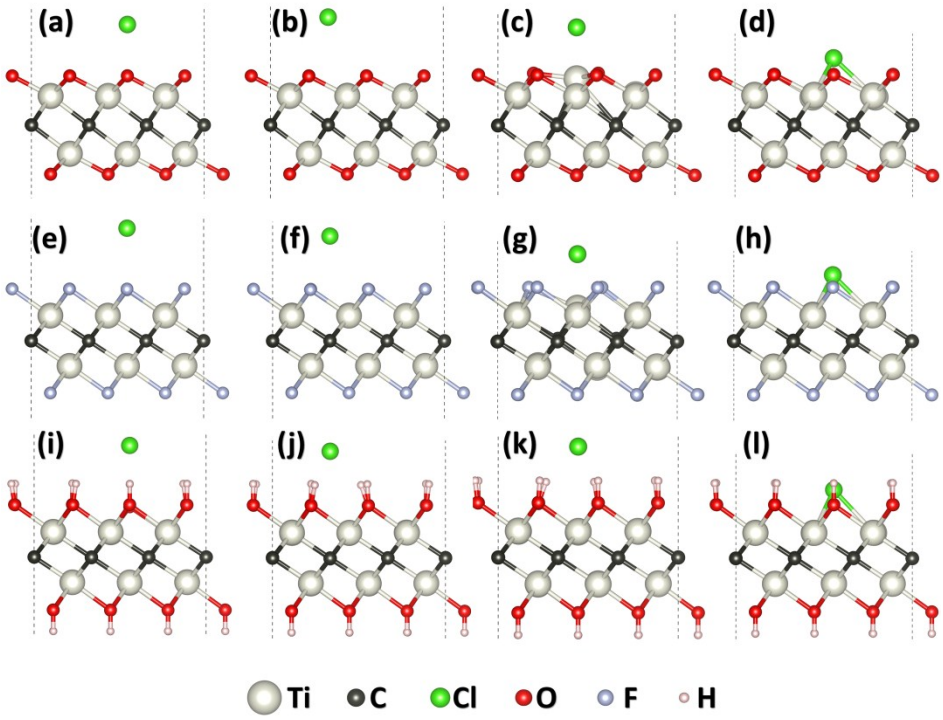

Fig. S3. Optimized Cl adsorption configurations for (a)–(d) Ti_2CO_2, (e)–(h) Ti_2CF_2, and (i)–(l) $Ti_2C(OH)_2$ monolayers. (d), (h), and (l) correspond to the Cl adsorption configurations on Ti_2CT_2 monolayers with one T (T = O, F, or OH, respectively) vacancy.

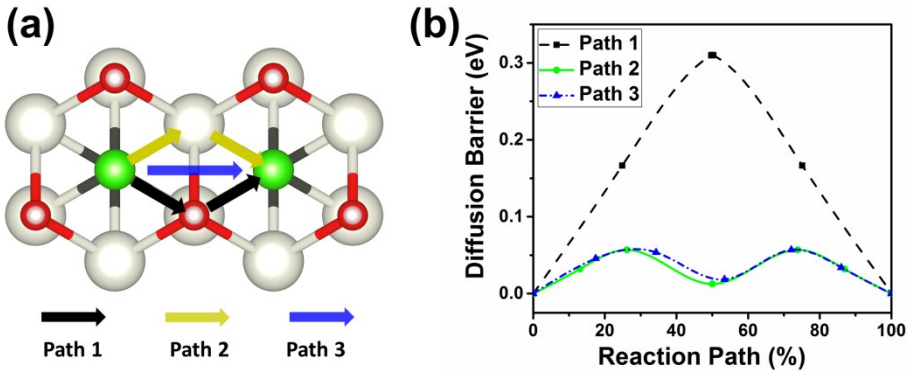

Fig. S4. (a)Possible Cl^- diffusion pathways on a $Ti_2C(OH)_2$ monolayer. (b) Diffusion barrier profiles of Cl^- on a $Ti_2C(OH)_2$ monolayer.