

Supporting Information

Scope, evaluation and current perspectives of MXene synthesis strategies for state of the art applications†

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S1. Effect of MXenes delamination via dimethyl sulfoxide

MXene synthesized via HF etchant and LiF/HCl (in-situ HF) etching, followed by delamination via dimethyl sulfoxide (DMSO), exhibits different surface terminations. In HF etching, O-terminations dominate on the MXene surfaces, making them suitable for water splitting, optical electronics, and water purification applications. On the other hand, in the in-situ HF method, OH terminations predominate, making it useful for energy storage and nuclear purification applications (see [Figure S1](#))[1].

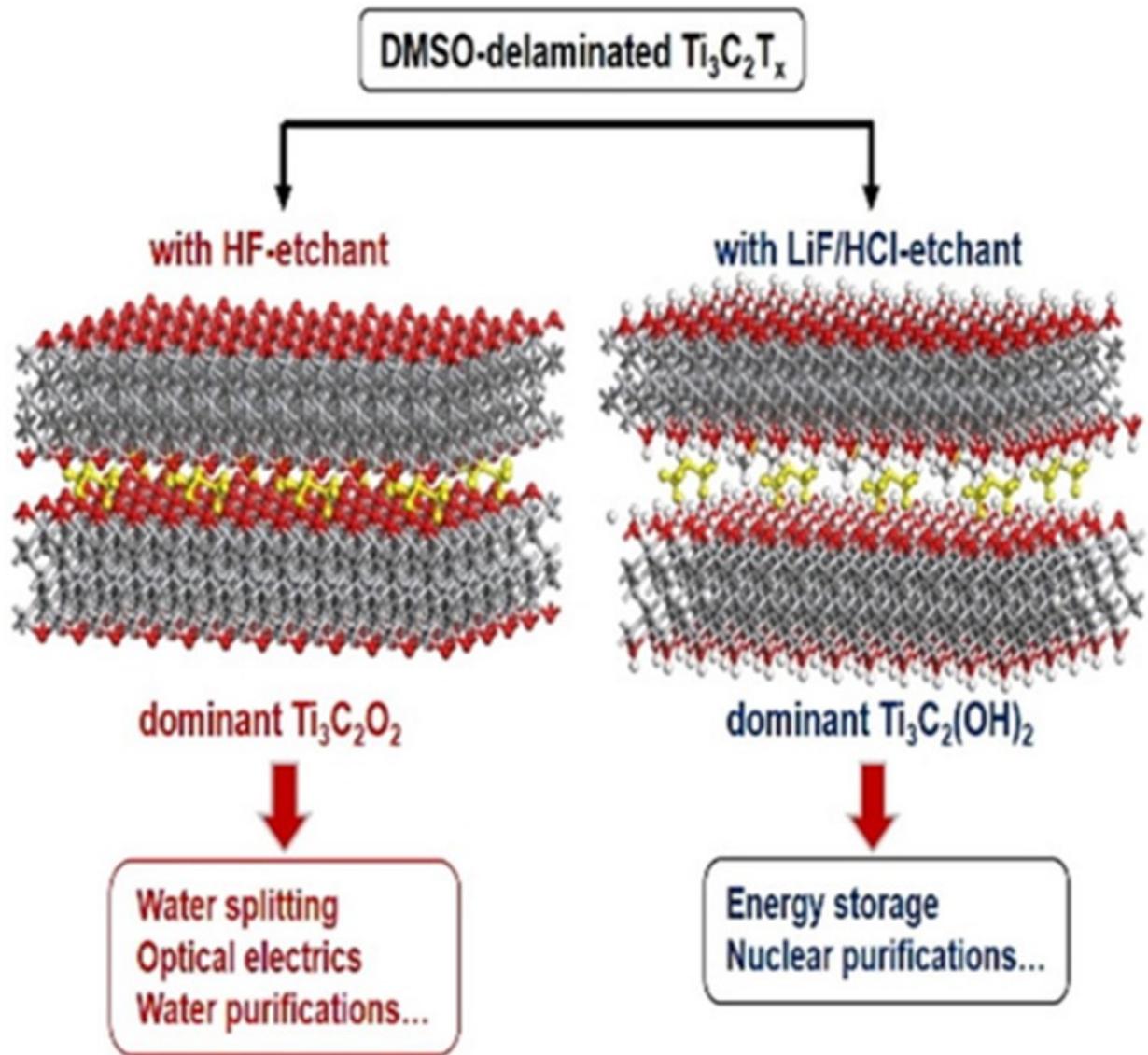


Figure S1: Effect of DMSO on delaminated $Ti_3C_2T_x$ [1].

The $\text{Ti}_3\text{C}_2\text{T}_x$ (LiF/HCl) samples exhibit considerable DMSO delamination effects when compared to non-delaminated $\text{Ti}_3\text{C}_2\text{T}_x$ (HF) samples, which have comparable O/F ratios of 1.37 and 1.42, but different O/F ratios of 2.9 and 3.6). Furthermore, despite having a lower equivalent series resistance, smaller interlayer spacing, and a slightly smaller specific surface area than delaminated $\text{Ti}_3\text{C}_2\text{T}_x$ (HF) samples, the delaminated $\text{Ti}_3\text{C}_2\text{T}_x$ (LiF/HCl) electrodes show a higher capacitance (see [Figure S2](#))[1].

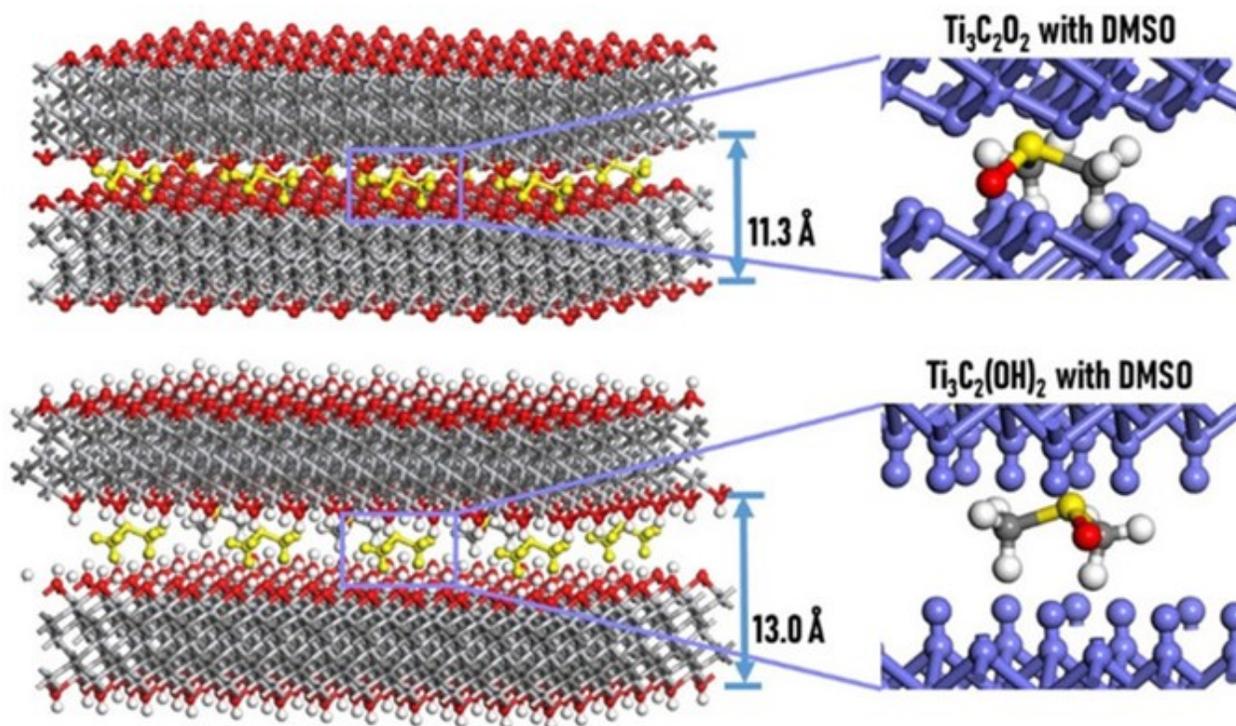


Figure S2: Structural calculation using DFT for O-terminated and OH-terminated delaminated MXene [1].

S2. Role of NH₂-terminations

To introduce the NH₂ terminations (amination), MXene along with ammonia was used to maintain pH 9 during the sealed thermal method. The synthesis process is illustrated in the Figure S3. As a result, MXene with terminations OH, NH₂, O, and F were produced[2]. The introduction of amino terminations altered the Zeta potential value, and the MXene-NH₂ exhibited excellent dispersity in water.

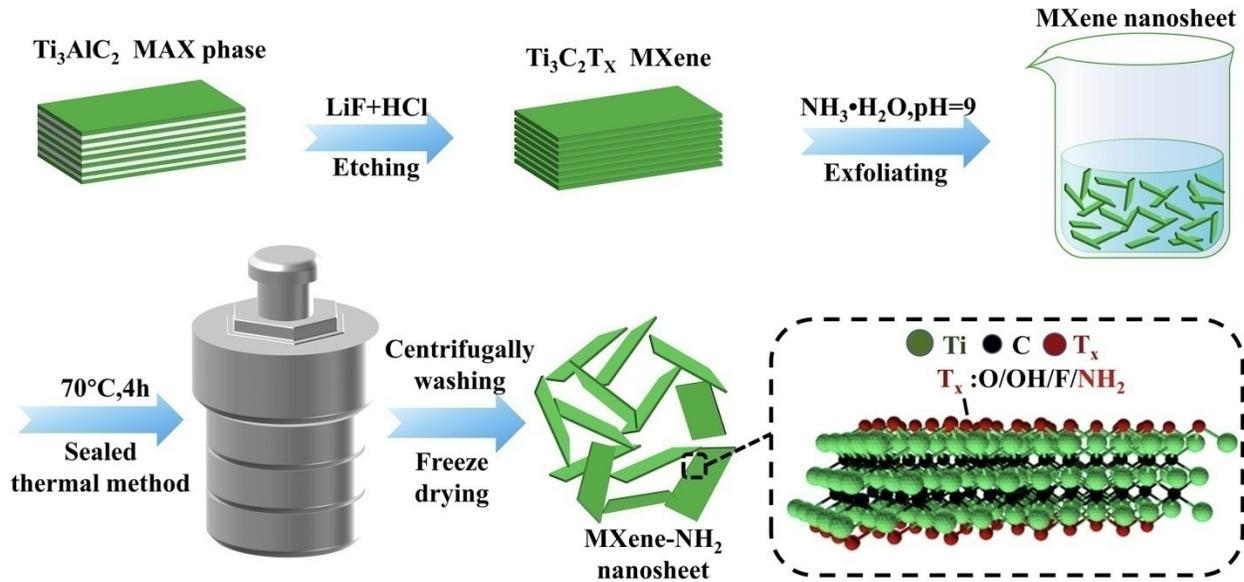


Figure S3: Schematic Illustration for introduction of NH₂-terminations over the Ti_3C_2 surface[2].

The mechanical properties of are primarily attributed to the hydrogen bonding between MXene and CMC. Moreover the covalent bond is formed through an amination reaction between carboxyl and amino groups. This additional covalent bonding, along with hydrogen bonding, led the CMC/MXene-NH₂ to greater flexibility and enhanced mechanical properties[2]. The mechanism for enhancing tensile strength is illustrated in Figure S4.

Interfacial shear τ

τ covalent bonding $>$ τ hydrogen bonding

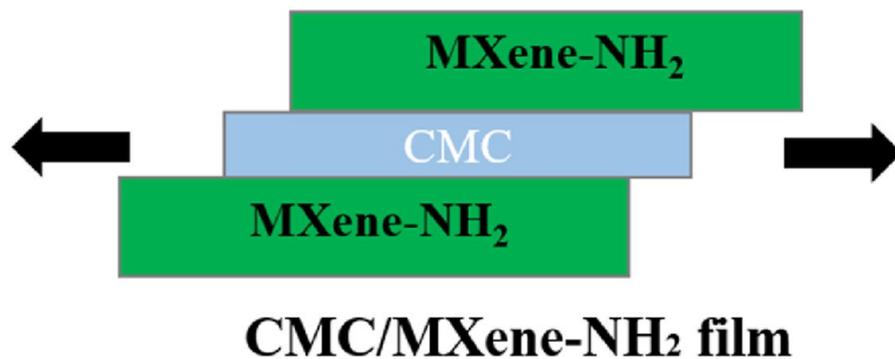


Figure S4: Illustration of mechanical strength mechanism [2].

S3. Effect of Lewis-basic halides on MXene

The Lewis-basic halide treatment is capable of simultaneously engineering the interlayer spacing and surface termination of various MXenes. The systematic illustration for Lewis-basic halide treatment of LB- $\text{Ti}_3\text{C}_2\text{T}_x$ is illustrated in [figure S5a](#). The interlayer gap was increased due to the desolvated Na^+ and K^+ ions that intercalate inside the $\text{Ti}_3\text{C}_2\text{T}_x$ layers during this process. Desolvated halogen anions (Br^-) are used to replace the surface F termination. A nucleophilic substitution takes place between the F atoms already present on the $\text{Ti}_3\text{C}_2\text{T}_x$ surface and the desolvated Br^- ions. The MXene surface is altered with bromine terminations as a result of this deliberate replacement operation. These chemical changes changed interlayer spacing and surface chemistry, improving its characteristics and prospective uses. The SEM results before and after these treatments are illustrated in the [Figure S5b](#)[3].

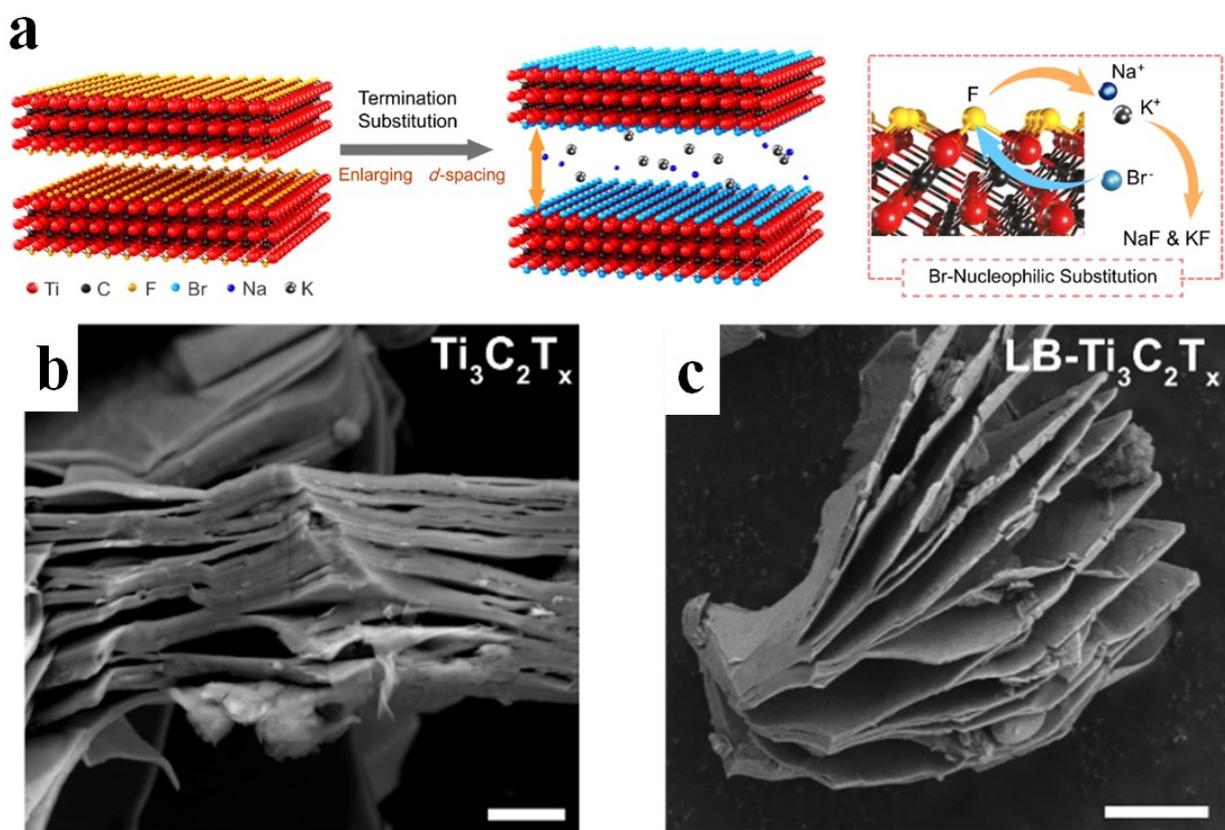


Figure S5:(a) Termination substitution and Lewis-basic halide treatment (b) MXene before treatment and (c) MXene after treatment [3].

S4. Role of Sulphur terminated MXenes

According to recent studies, S-terminated MXenes have potential to be utilized as anode material. According to Metha et al. [4], S-terminated Mo_2C (MXene) significantly boosts the Li adsorption capacity. Yan et al. discovered low barriers of 0.15 and 0.22 eV for the transport of lithium (Li) atoms in V_2CT_x ($T_x = \text{O}$ and S) [5], leading to a high theoretical capacity (367.64 and 301.22 mAh/g)[6]. Wang et al. conducted simulations and found that an S-terminated $\text{Ti}_3\text{C}_2\text{S}_2$ can effectively absorb Na-ion, resulting in a higher theoretical capacity 463 mAh/g compared to bare Ti_3C_2 . Moreover, the S-terminated Ti_2C demonstrated promising theoretical capacities of 935.57 mAh/g in Na-ion batteries and 1871.13 mAh/g in Mg-ion batteries [6]. The schematic illustration of $\text{MoS}_2/\text{Mo}_2\text{TiC}_2\text{T}_x$ heterostructures was illustrated in [Figure S6a](#). The comparison of different functionalized (N, O, F, S, Cl) Ti_3C_2 displays distinct adsorption strengths during lithiation as illustrated in [Figure S6b](#). Specifically, the strength follows the sequence $\text{Ti}_3\text{C}_2\text{Cl}_2 < \text{Ti}_3\text{C}_2\text{F}_2 < \text{Ti}_3\text{C}_2\text{N}_2 < \text{Ti}_3\text{C}_2\text{O}_2 < \text{Ti}_3\text{C}_2\text{S}_2$. The adsorption strength of various sulfur species increases as the lithium content rises, this finding underscores the effective anchoring effect of $\text{Ti}_3\text{C}_2\text{S}_2$, which significantly suppresses the migration of polysulfides. These conclusions highlight the strategic role played by surface-modified MXenes, paving the way for enhanced battery performance and durability[7].

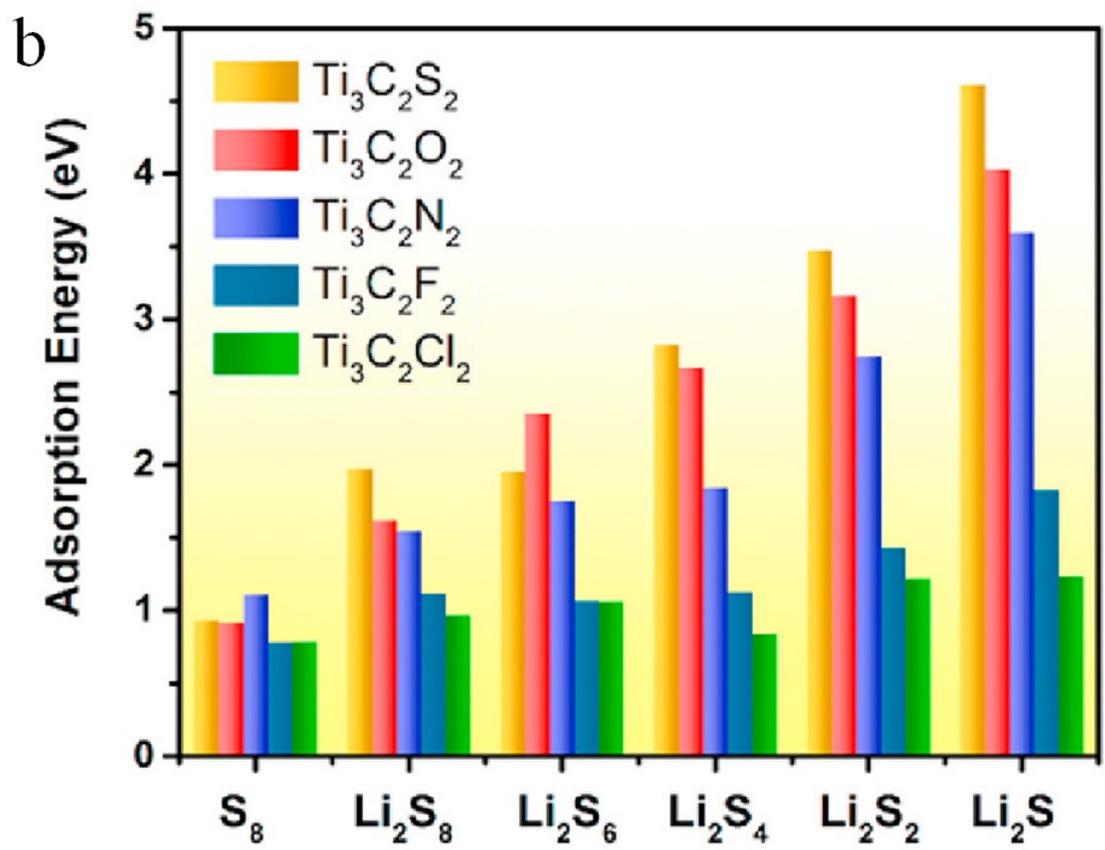
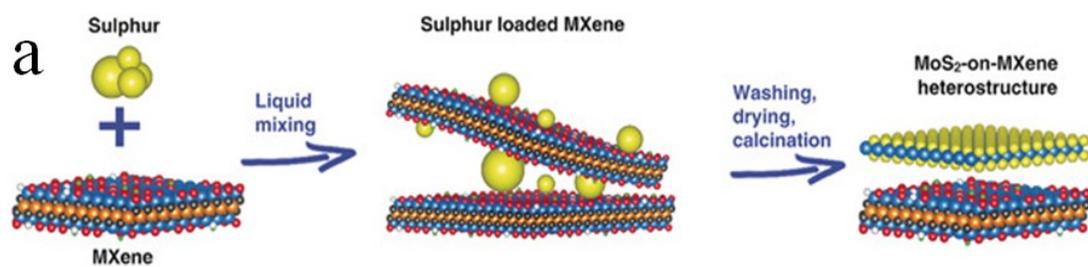


Figure S6:(a) Illustration of in-situ sulfidation of Mo₂TiC₂T_x MXene[8].Binding energies between the S species and various functionalized (N, O, F, S, Cl) Ti₃C₂ MXenes[7].

S5. Mechanism for the removal of toxic metals via MXenes

MXene demonstrates that a larger interlayer space and exhibits flexibility and swelling properties that enable it to efficiently accommodate a higher number of metal ions. It is important to understand the physical and chemical interaction mechanisms. These mechanisms differ depending on the adsorbent materials employed and vary between different heavy metals. The mechanism primarily involves electrostatic interactions, ion exchange, and surface complexation [9](See Figure S7).

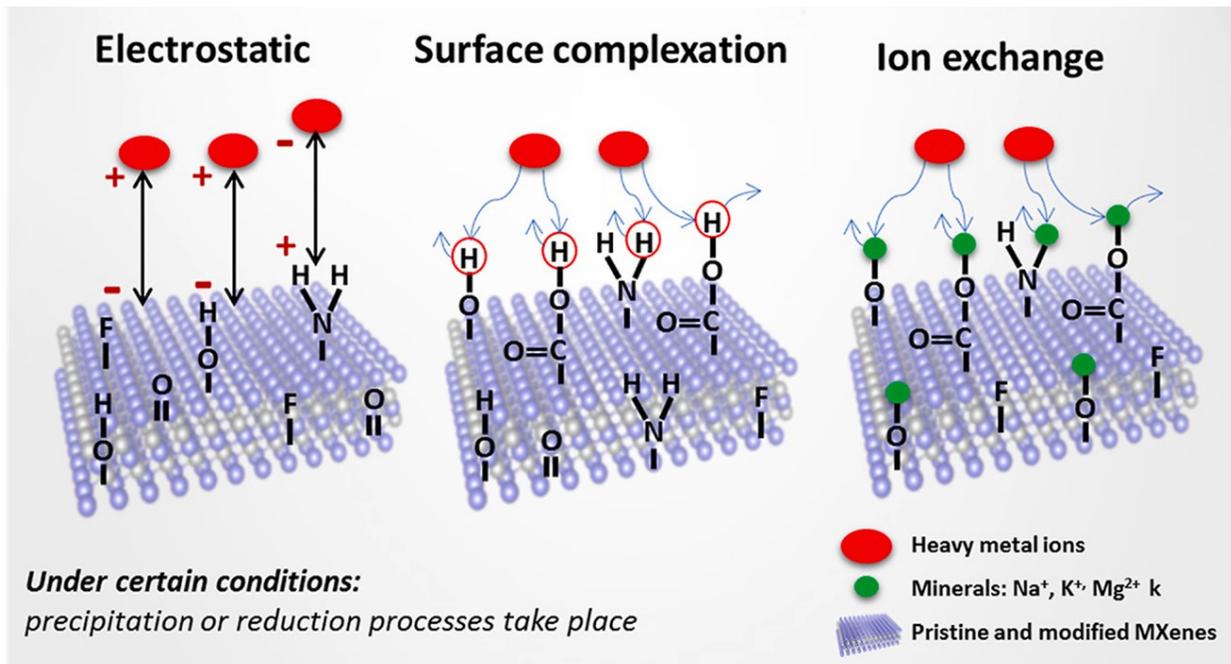


Figure S7: Mechanism of adsorption on MXene surface [9].

References:

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