Supporting Information

First-principles calculation on the lithium storage properties of high-entropy MXene $Ti_3C_2(N_{0.25}O_{0.25}F_{0.25}S_{0.25})_2$

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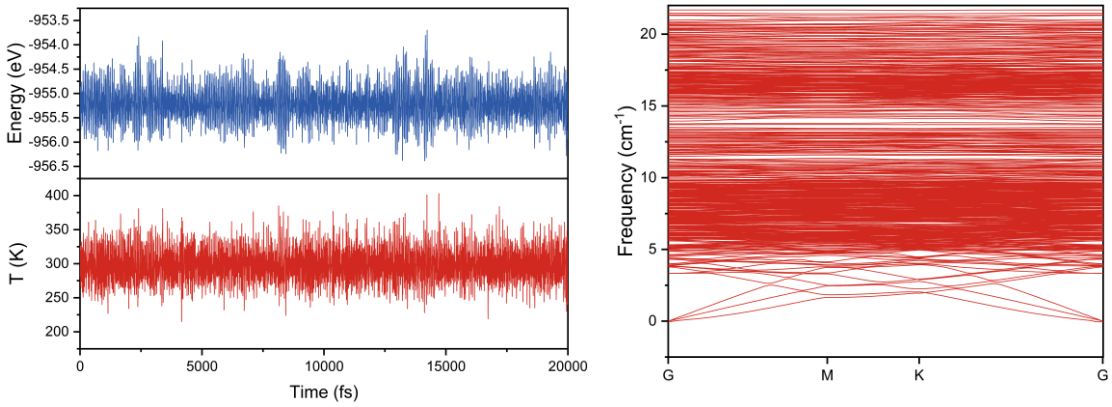

Fig. S1 (a) AIMD simulation of the total energy and temperature profiles of $Ti_3C_2(N_{0.25}O_{0.25}F_{0.25}S_{0.25})_2$ monolayer at 300K. (b) Phonon dispersion spectra of $Ti_3C_2(N_{0.25}O_{0.25}F_{0.25}S_{0.25})_2$ monolayer.

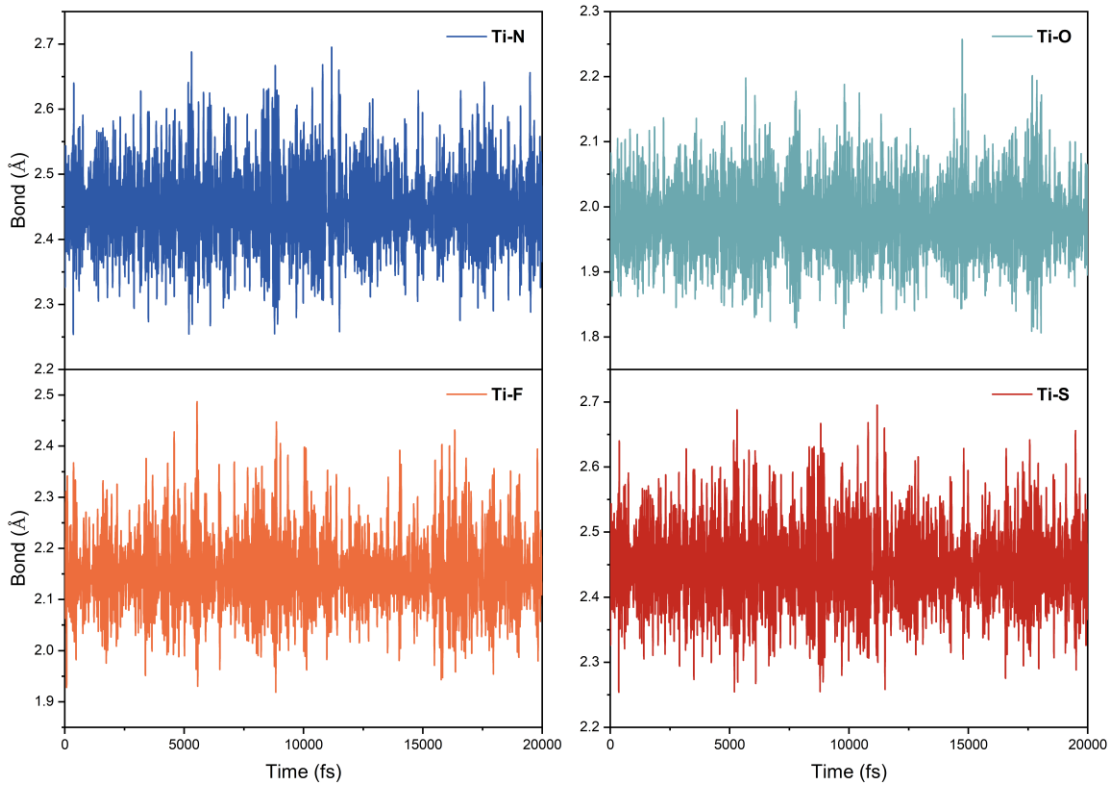

Fig. S2 AIMD simulation of the Ti-N, Ti-O, Ti-F, and Ti-S bonds of $Ti_3C_2(N_{0.25}O_{0.25}F_{0.25}S_{0.25})_2$ monolayer with their length change at 300K.

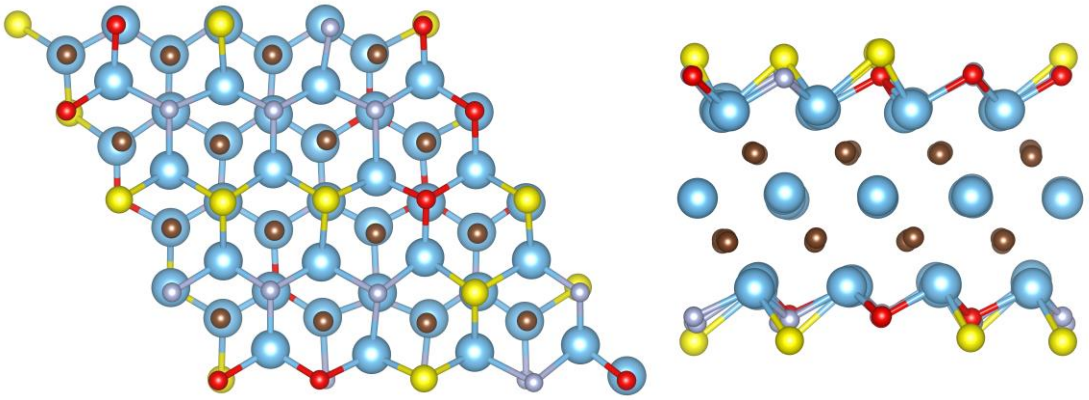

Fig. S3 Schematic diagram of material structure after AIMD simulation at 300K temperature.

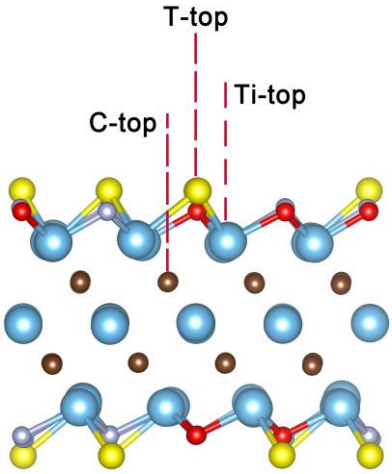

Fig. S4 Side view of the possible adsorption sites for Li-ion on $Ti_3C_2(N_{0.25}O_{0.25}F_{0.25}S_{0.25})_2$ surface.

Table S1 The adsorption energy at the adsorption position of A-side and the corresponding charge transfer of the Li atom

Adsorption site	Adsorption Energy (eV)	q (e)
C1	-2.62	-0.88
C2	-2.40	-0.88
C3	-2.47	-0.88
C4	-2.30	-0.90
C5	-2.35	-0.89
C6	-2.52	-0.88
C7	-2.45	-0.88
C8	-2.42	-0.89
C9	-2.64	-0.87
C10	-2.66	-0.87
C11	-2.46	-0.89
C12	-2.49	-0.88
C13	-2.86	-0.87
C14	-2.62	-0.88
C15	-2.25	-0.88
C16	-2.49	-0.88
Ti1	→C1	-
Ti2	→C6	-
Ti3	-2.19	-0.88
Ti4	→C1	-
Ti5	-2.25	-0.88
Ti6	-2.50	-0.89
Ti7	-2.31	-0.89
Ti8	-2.40	-0.89
Ti9	→C13	-
Ti10	-2.46	-0.89
Ti11	-2.46	-0.89
Ti12	→C9	-0.87
Ti13	-2.37	-0.90
Ti14	→C14	-0.89
Ti15	-2.20	-0.89
Ti16	→C13	-

Table S2 The adsorption energy at the adsorption position of B-side and the corresponding charge transfer of the Li atom

Adsorption site	Adsorption Energy (eV)	q (e)
C1	-2.35	-0.89
C2	-2.01	-0.90
C3	-2.68	-0.88
C4	-2.69	-0.87
C5	-2.76	-0.87
C6	-2.58	-0.88
C7	-2.56	-0.88
C8	-2.70	-0.87
C9	-2.58	-0.89
C10	-3.16	-0.86
C11	-2.76	-0.88
C12	-2.57	-0.88
C13	-2.11	-0.89
C14	-2.44	-0.89
C15	-2.98	-0.87
C16	-2.56	-0.88
Ti1	-2.49	-0.88
Ti2	-2.11	-0.91
Ti3	-2.17	-0.90
Ti4	-2.63	-0.89
Ti5	-2.57	-0.89
Ti6	→C10	-
Ti7	→C11	-
Ti8	-2.70	-0.87
Ti9	→C9	-
Ti10	→C10	-
Ti11	-2.55	-0.90
Ti12	→C11	-
Ti13	-2.14	-0.89
Ti14	-1.92	-0.91
Ti15	→C15	-
Ti16	→C15	-