Supporting Information

Structural Engineering of MXenes for Enhanced Magnesium Ion Diffusion: A Computational Study

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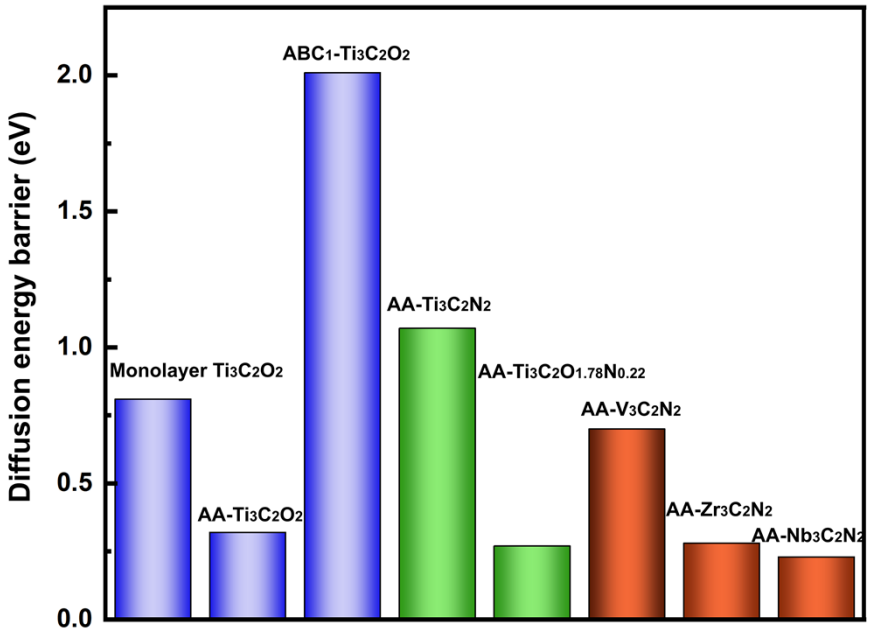

Figure S1. The migration energy barrier of all structures.

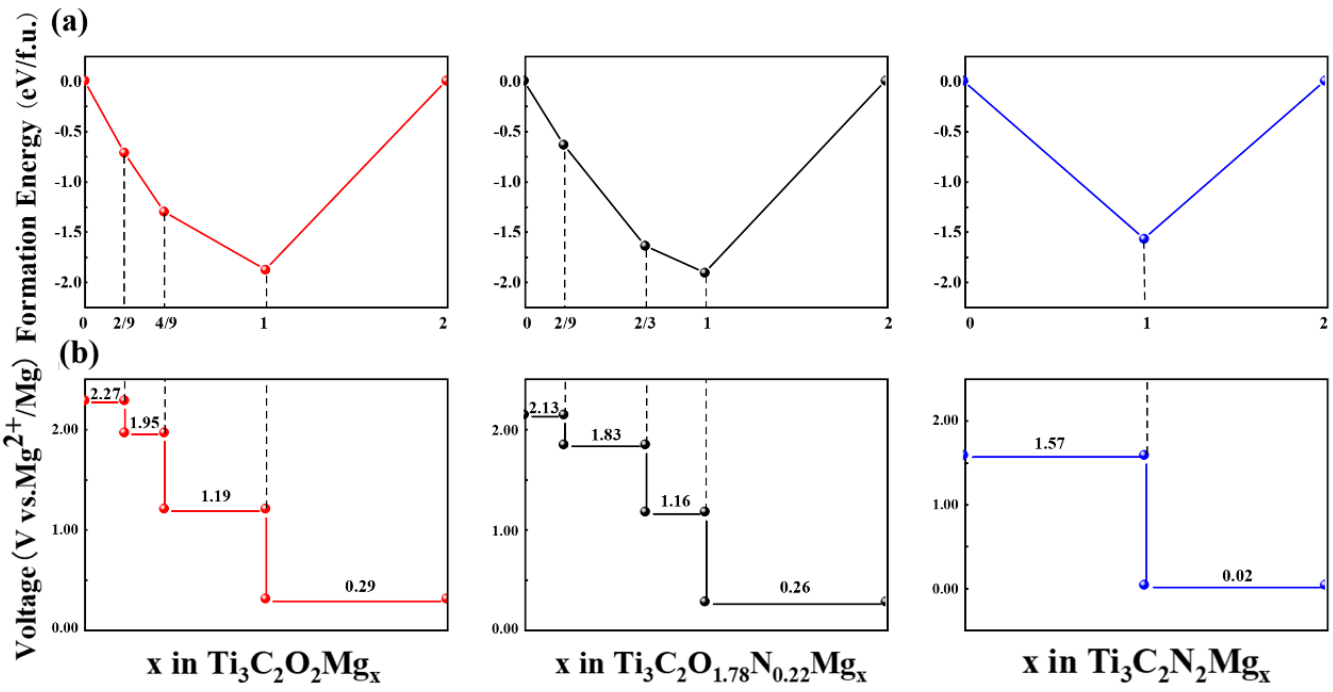

Figure S2. (a) Convex hull of formation energy vs. Mg^{2+} concentration (x) for $Ti_3C_2O_2Mg_x$, $Ti_3C_2O_{1.78}N_{0.22}Mg_x$ and $Ti_3C_2N_2Mg_x$. (b) The voltage plateaus vs. Mg^{2+}/Mg.

Table S1. Calculated lattice parameters and atomic positions of AA-type $Ti_3C_2O_2$.

AA-type $Ti_3C_2O_2$ (164 -- P-3m1)				
a = 3.025 Å; b = 3.025 Å; c = 9.803 Å; V = 77.692 $Å^3$; α = β =90° ;γ = 120°				
atom	Wychoff	x	y	z
Ti (1)	2d	0.333	0.667	0.239
Ti (2)	1b	-0.000	3.000	0.500
C (1)	2d	0.333	0.667	0.627
O (1)	2c	0.000	3.000	0.855

Table S2. Calculated lattice parameters and atomic positions of ABC_1-type $Ti_3C_2O_2$.

ABC_1-type $Ti_3C_2O_2$ (166 -- R-3m)				
a = 3.031 Å; b = 3.031 Å; c = 27.901 Å; V = 221.972 $Å^3$; α = β =90° ;γ = 120°				
atom	Wychoff	x	y	z
Ti (1)	6c	0.333	0.667	-0.092
Ti (2)	3a	0.000	0.000	0.000
C (1)	6c	0.333	0.667	0.045
O (1)	6c	0.000	1.000	0.124

Table S3. Calculated lattice parameters and atomic positions of ABC_2-type $Ti_3C_2O_2$.

ABC_2-type $Ti_3C_2O_2$ (166 -- R-3m)				
a = 3.026 Å; b = 3.026 Å; c = 28.418 Å; V = 225.337 $Å^3$; α = β =90° ;γ = 120°				
atom	Wychoff	x	y	z
Ti (1)	6c	-0.333	-0.667	-0.090
Ti (2)	3a	-3.000	-0.000	0.000
C (1)	6c	-0.333	0.667	0.045
O (1)	6c	-3.000	-0.000	0.122