Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Exploring the possibilities of two dimensional transition metal carbides as anode material for sodium batteries

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Table S1. Computed total energy differences of O termination types relative to the most stable configuration (bold typeface) in eV. For M = Ti and Ni, the hcp-type O termination relaxed to the fcc-type structure after geometry optimization. 1×1 unit cell was used for the calculations.

M in M_2CO_2	fcc-type	hcp-type	Mixed-type
Ti	**0.000**	-	0.757
V	**0.000**	0.608	0.260
Cr	0.193	**0.000**	0.128
Mn	**0.000**	0.336	0.430
Fe	**0.000**	0.284	0.199
Co	**0.000**	0.829	0.468
Ni	**0.000**	-	0.480
Nb	**0.000**	0.503	0.158
Mo	1.087	**0.000**	0.677

Table S2. Average Bader charges based on the electronic charge density of bare (M_2CO_2), lithiated ($M_2CO_2Li_2$), and sodiated ($M_2CO_2Na_2$) MXene sheets.

		M	C	O	Li or Na
Ti	Bare	1.56	-1.18	-0.97	
	Lithiated	1.25	-1.21	-0.83	0.18
	Sodiated	1.36	-1.20	-1.05	0.30
V	Bare	1.45	-1.12	-0.90	
	Lithiated	1.19	-1.13	-0.80	0.18
	Sodiated	1.27	-1.12	-1.02	0.32
Cr	Bare	1.24	-0.97	-0.76	
	Lithiated	1.10	-1.01	-0.75	0.16
	Sodiated	1.16	-0.98	-0.95	0.28
Mn	Bare	1.30	-0.92	-0.84	
	Lithiated	0.96	-0.86	-1.18	0.65
	Sodiated	1.63	-1.64	-1.71	0.90
Fe	Bare	1.10	-0.73	-0.73	
	Lithiated	0.74	-0.59	-1.14	0.70
	Sodiated	1.38	-1.34	-1.63	0.92
Co	Bare	0.89	-0.53	-0.62	
	Lithiated	0.53	-0.35	-1.07	0.72
	Sodiated	1.13	-1.02	-1.54	0.92
Ni	Bare	0.70	-0.27	-0.57	
	Lithiated	0.50	-0.27	-1.04	0.68
	Sodiated	1.02	-0.84	-1.53	0.93
Nb	Bare	2.21	-1.81	-1.30	
	Lithiated	1.78	-1.86	-1.03	0.19
	Sodiated	1.78	-1.86	-1.04	0.19
Mo	Bare	1.82	-1.52	-1.06	
	Lithiated	1.57	-1.58	-0.94	0.17
	Sodiated	1.68	-1.54	-1.18	0.27

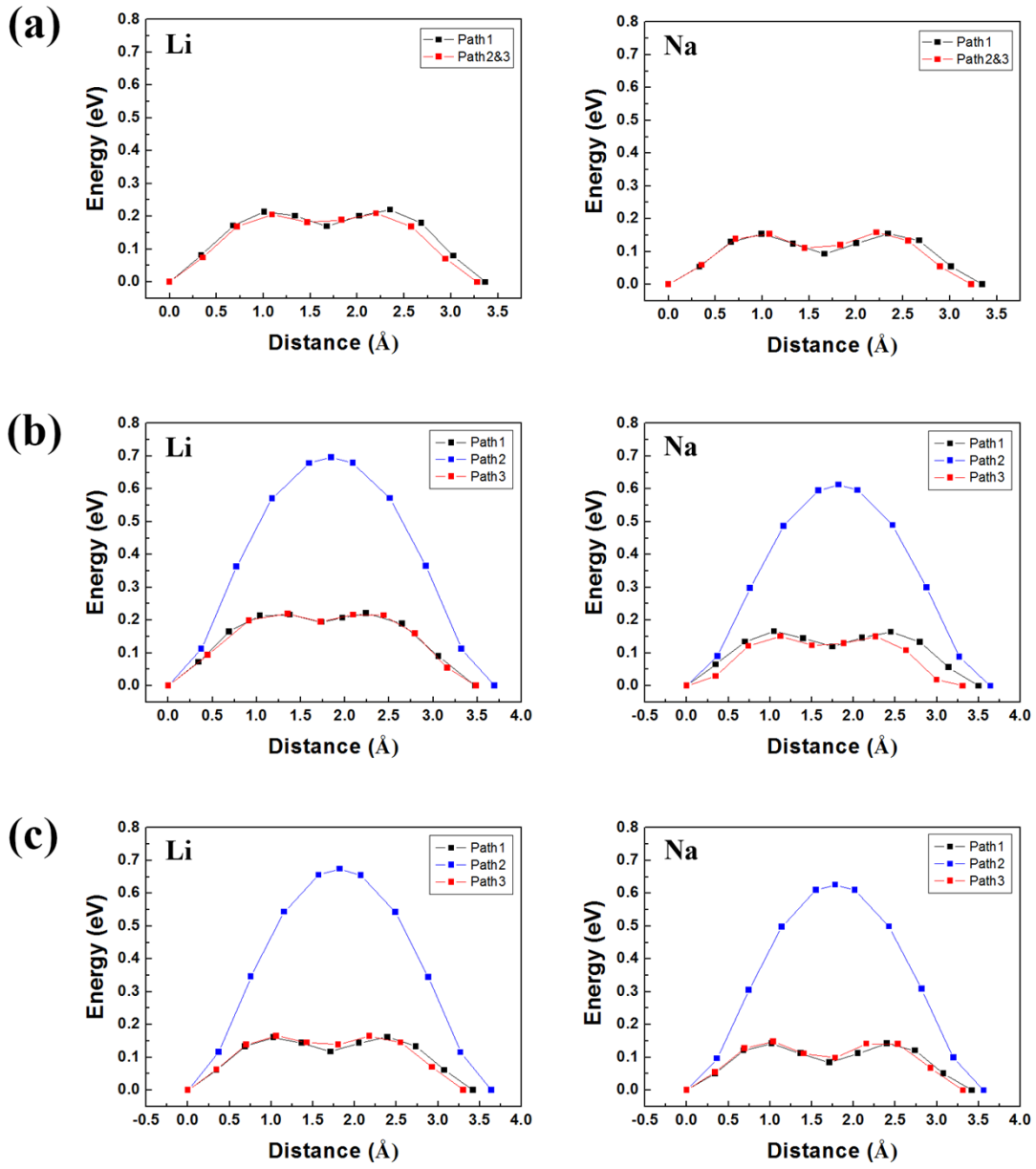

Figure S1. Considered ion migration pathways and corresponding energy profiles of Li and Na on (a) V_2CO_2, (b) Mn_2CO_2, and (c) Mo_2CO_2.