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Theoretical prediction of MXene-like structure Ti_3C_4 as a high capacity electrode material for Na ion batteries

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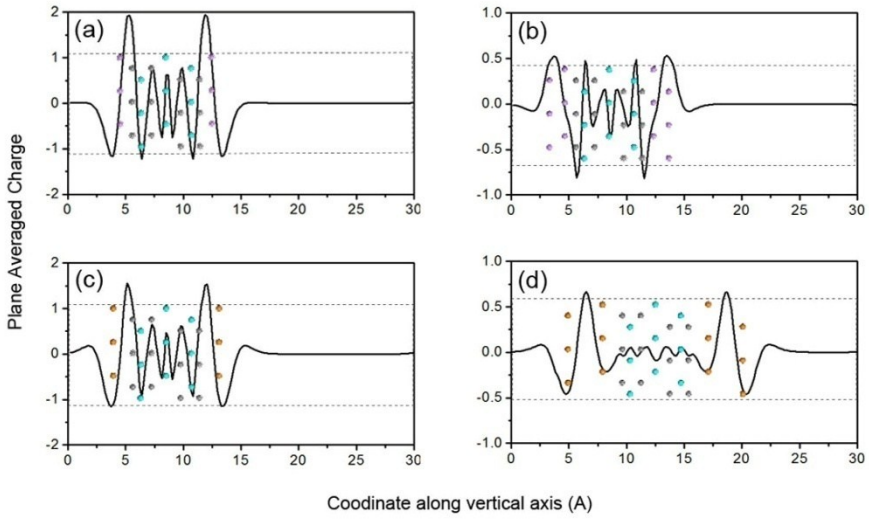

Figure S1. Difference charge transfer of plane averaged charge for (a-b) $Ti_3C_4Li_2$ monolayer, and with an extra Li layer; (c-d) $Ti_3C_4Na_2$ monolayer, and with an extra Na layer, respectively.

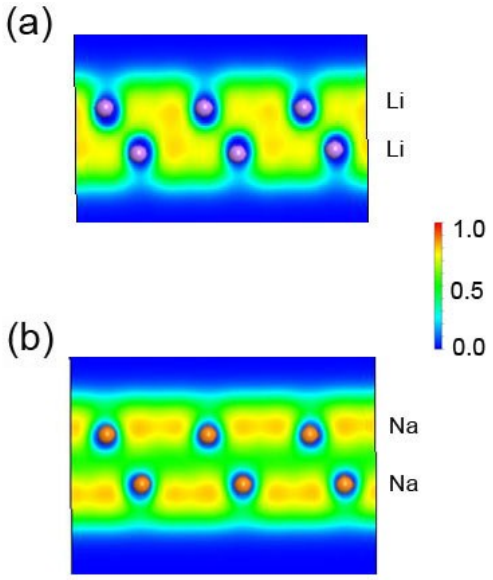

Figure S2. The electron localization functions of the (110) section of (a) the Li bilayer; and (b) the Na bilayer, respectively.

TableS1. The relative energies with respect to the lowest energy electrically neutral system of Li and Na monolayer and bilayer by adding and subtracting one electron, respectively.

	Electrically neutral (eV/atom)	Negative (eV/atom)	Positive (eV/atom)
Li monolayer	0	-0.194	0.537
Li bilayer	0	-0.093	0.219
Na monolayer	0	-0.149	0.463
Na bilayer	0	-0.065	0.179