Supplementary Information

Two-Dimensional Titanium Carbide ($Ti_3C_2T_x$) MXenes to Inhibit the Shuttle Effect in Sodium Sulfur Batteries

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Table S1. Optimized structural parameters for the $Ti_3C_2F_2$ and $Ti_3C_2O_2$ Mxenes monosheets

Formula	Lattice parameters (Å)		Bond lengths (Å)	
$Ti_3C_2F_2$	a	3.053	Ti1-C	2.071
	b	3.053	Ti2-C	2.183
	c	21.065	Ti1-F	2.162
	d	13.813	Ti1-Ti2	2.958
$Ti_3C_2O_2$	a	3.047	Ti1-C	2.197
	b	3.046	Ti2-C	2.162
	c	21.152	Ti1-O	1.983
	d	14.169	Ti1-Ti2	3.118

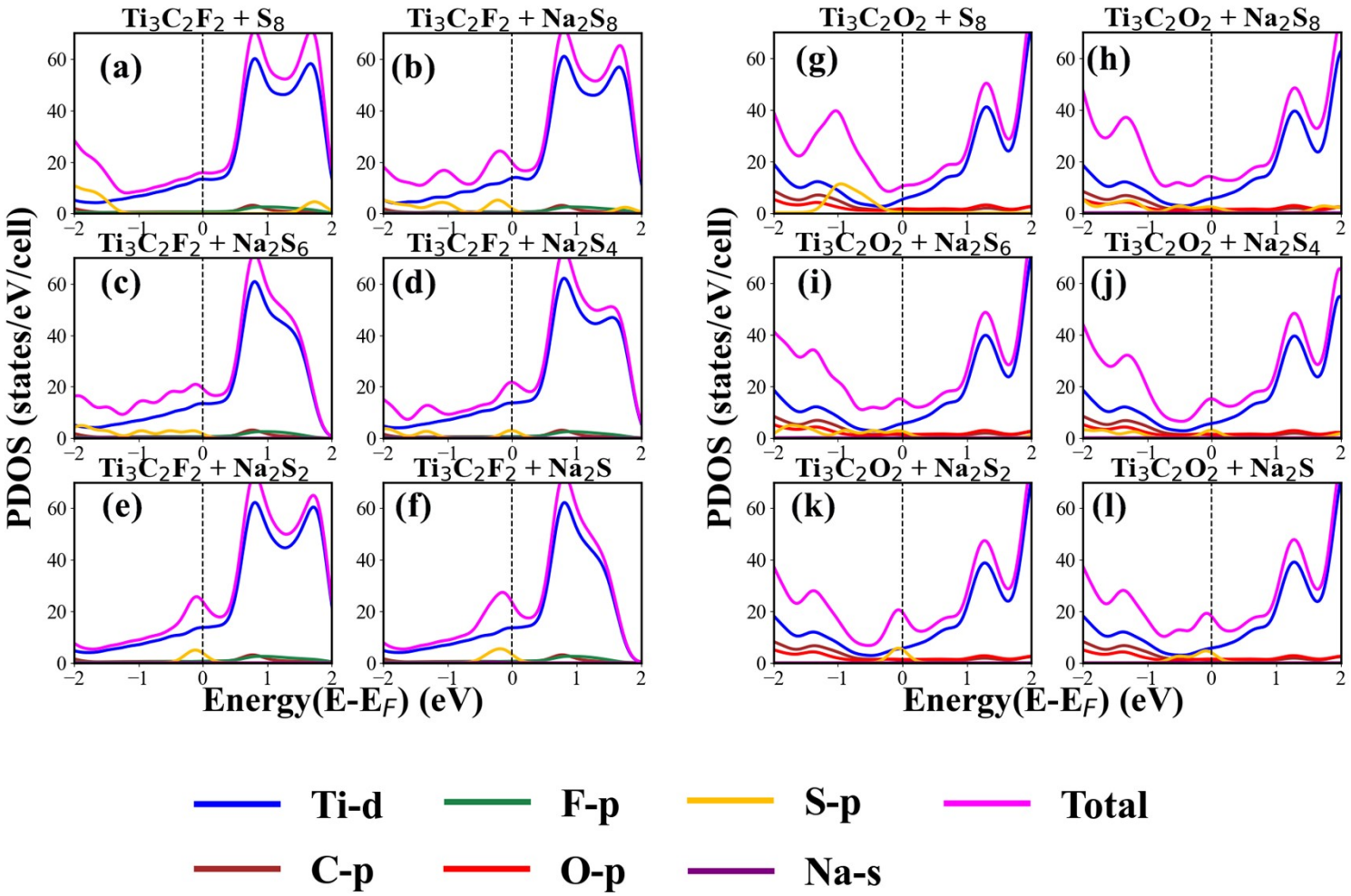

Figure S1. PDOS of (a-f) Na_2S_n – adsorbed $Ti_3C_2F_2$ and (g-l) Na_2S_n – adsorbed $Ti_3C_2O_2$. The Fermi energy has been shifted to zero