Electronic Supplementary Material (ESI)

Covalent Surface Modifications of Bifunctional Two-dimensional Metal Carbide MXenes as Sulfur Hosts for Sodium−Sulfur Batteries

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SI-1: The Effect of the Size of MXene Supercell on the Binding Energies of S Species

Many previous works employed 4 ×4 ×1 MXene supercell to study the interactions between LiPSs/NaPSs and MXenes and obtained reliable and reasonable results[1-4]. In order to verify the reasonability of the 4 ×4 ×1 supercell, here, we compared the binding energies (E_b) of Na_2S_8, Na_2S_6, and Na_2S_4 on 4 ×4 ×1 and 5 ×5 ×1 MXene supercell, respectively. As shown in Table S1, E_b of these NaPSs calculated by using 4 ×4 ×1 supercell is very close to 5×5 ×1 supercell, implying that 4 ×4 ×1 MXene supercell is large enough to eliminate the interactions from the periodic images.

Table S1 Binding energies (E_b, eV) of Na_2S_8, Na_2S_6, and Na_2S_4 adsorbed on 4 ×4 ×1 and 5 ×5 ×1 Ti_2CO_2 supercells, respectively

	E_b (Na_2S_8)	E_b (Na_2S_6)	E_b (Na_2S_4)
4 ×4 ×1	1.707	1.561	2.482
5 ×5 ×1	1.700	1.570	2.502

SI-2: Confirmation of the Most Favourable Adsorption Configuration of Various NaPSs over Ti_2CO_2

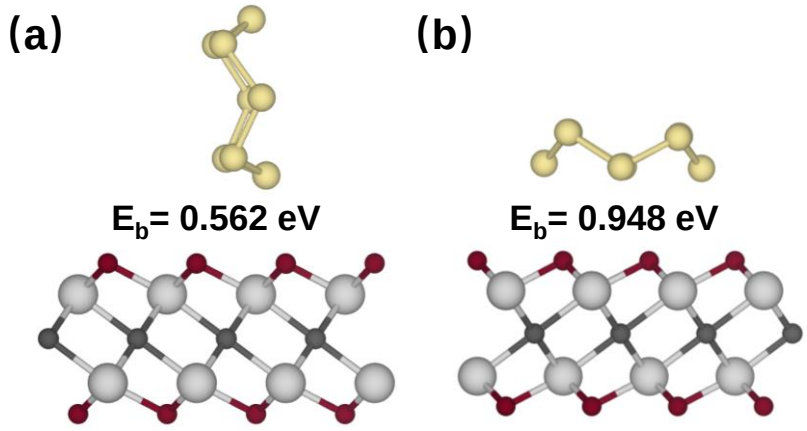

Figure S1. Optimized geometries of possible adsorption configurations of S_8 on Ti_2CO_2 (a-b), and the calculated binding energies (E_b in eV) are also given.

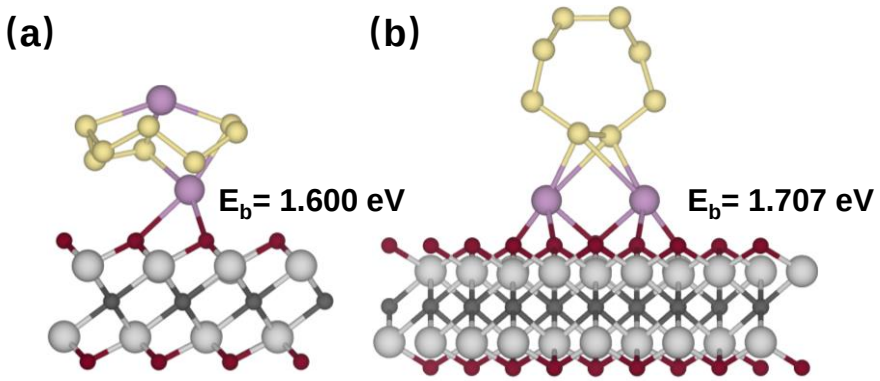

Figure S2. Optimized geometries of possible adsorption configurations of Na_2S_8 on Ti_2CO_2 (a-b), and the calculated binding energies (E_b in eV) are also given.

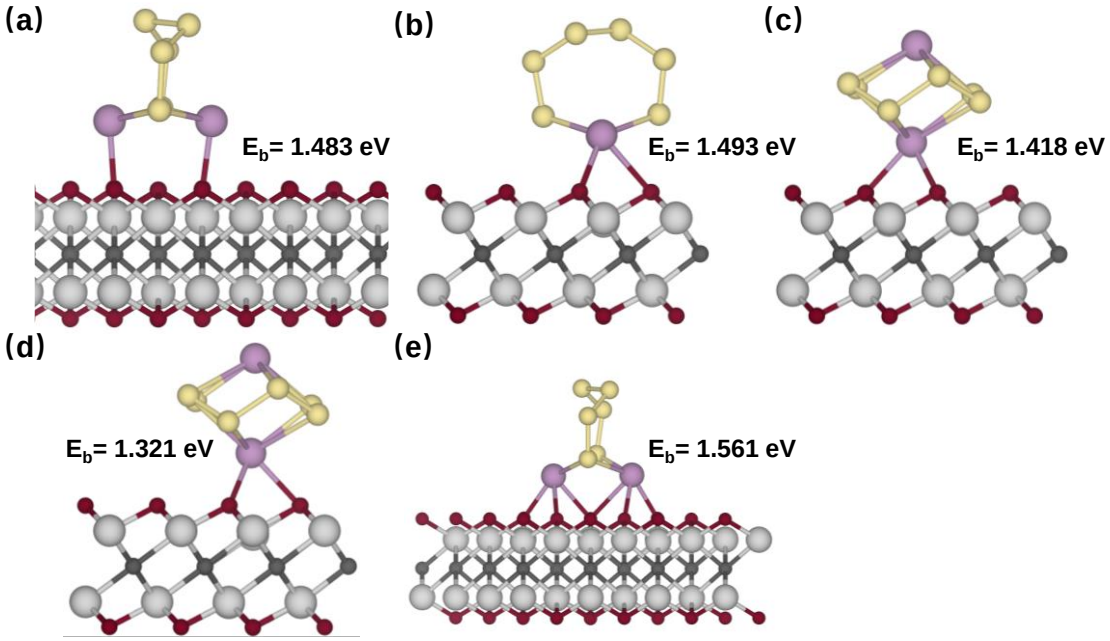

Figure S3. Optimized geometries of possible adsorption configurations of Na_2S_6 on Ti_2CO_2 (a-e), and the calculated binding energies (E_b in eV) are also given.

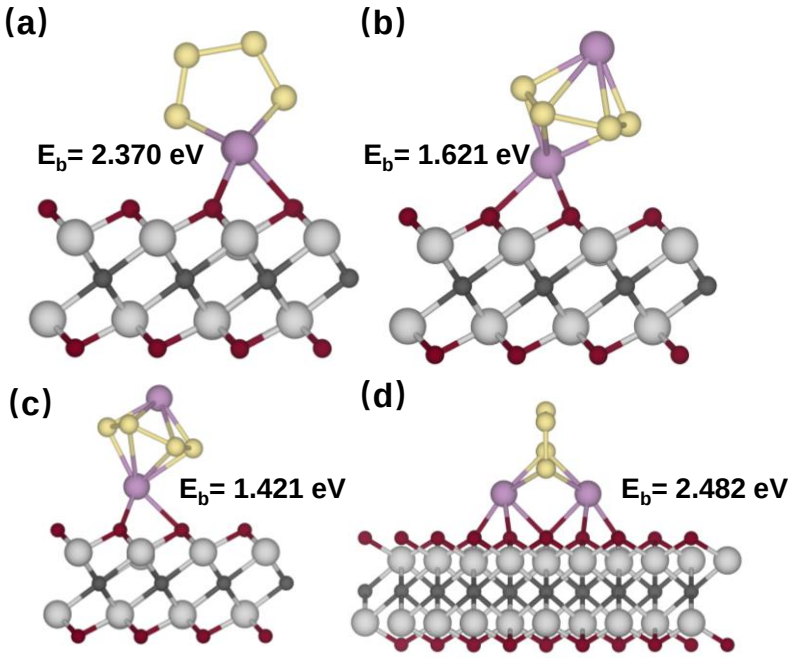

Figure S4. Optimized geometries of possible adsorption configurations of Na_2S_4 on Ti_2CO_2 (a-d), and the calculated binding energies (E_b in eV) are also given.

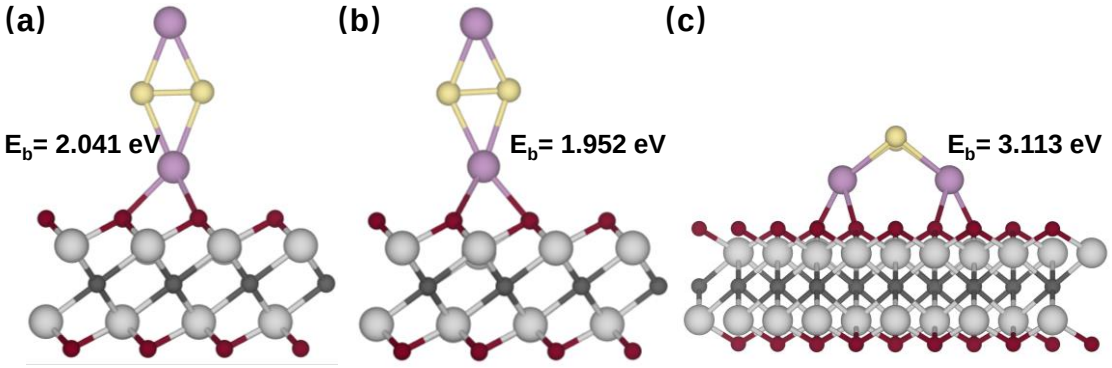

Figure S5. Optimized geometries of possible adsorption configurations of Na_2S_2 on Ti_2CO_2 (a-c), and the calculated binding energies (E_b in eV) are also given.

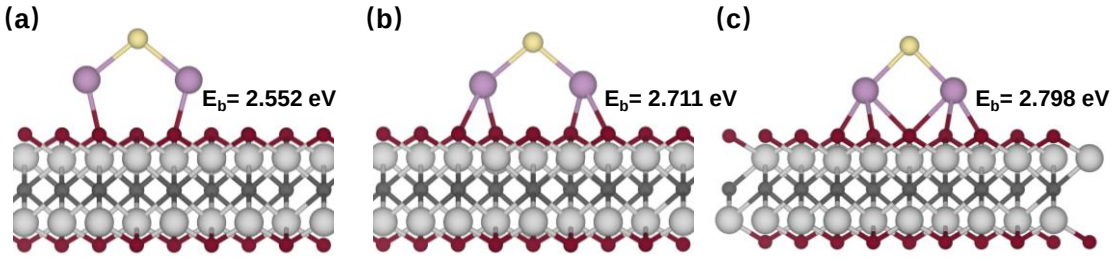

Figure S6. Optimized geometries of possible adsorption configurations of Na_2S on Ti_2CO_2 (a-c), and the calculated binding energies (E_b in eV) are also given.

SI-3: Interactions between Soluble NaPSs and Organic Electrolyte

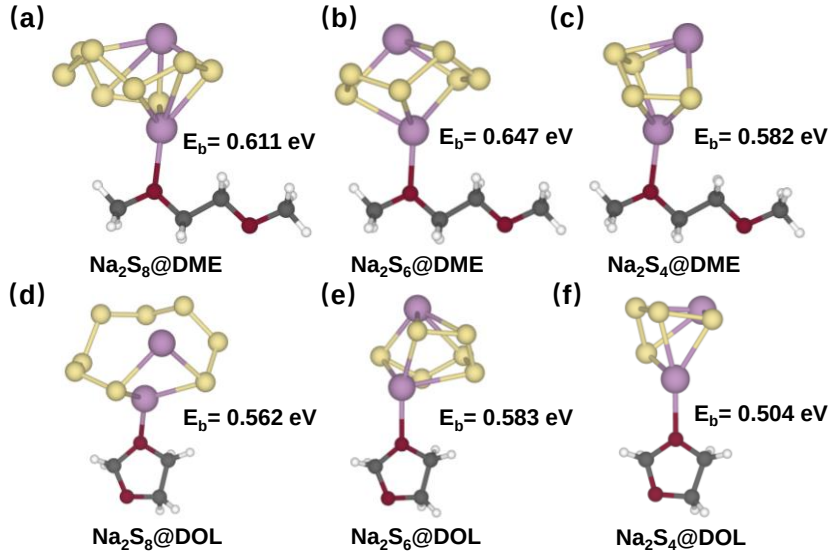

Figure S7. Optimized adsorption configurations and binding energies of Na_2S_8, Na_2S_6, and Na_2S_4 on DME (a-c) and DOL (d-f).

SI-4: Density of states (DOS) of S_8/Na_2S_x Adsorbed on Ti_2CS_2 and Ti_2CN_2

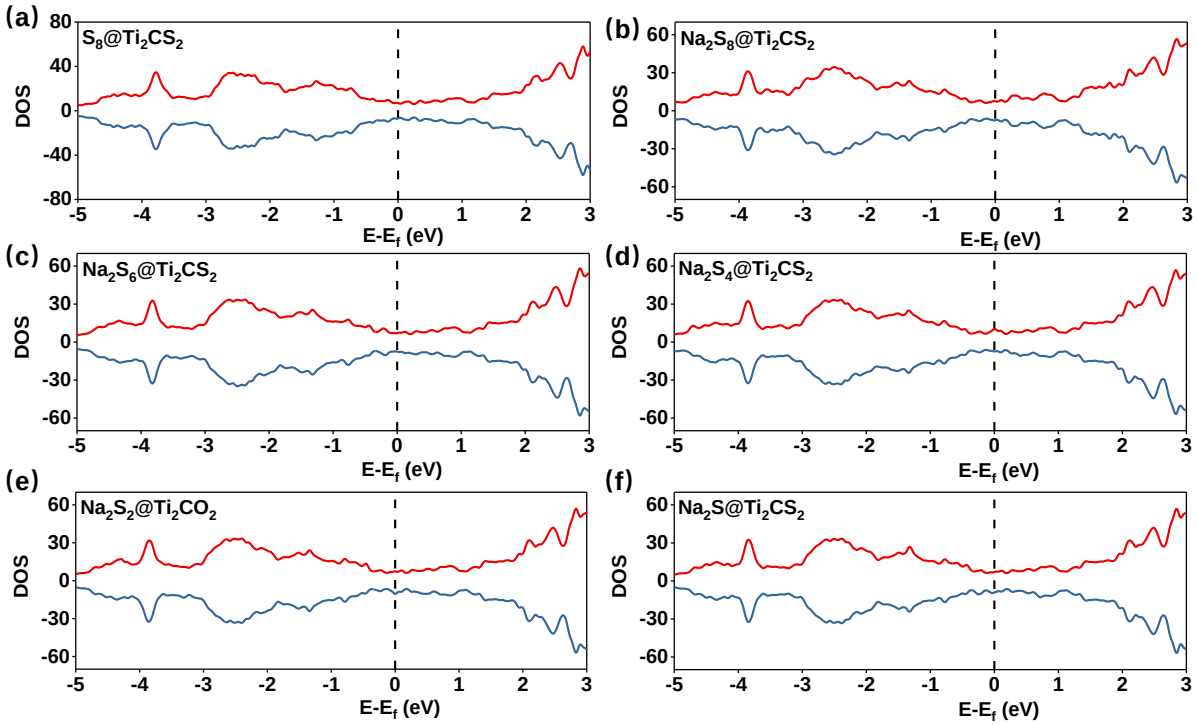

Figure S8. Total density of states (TDOS) of S_8 (a), Na_2S_8 (b), Na_2S_6 (c), Na_2S_4 (d), Na_2S_2 (e), and Na_2S (f) adsorbed on Ti_2CS_2.

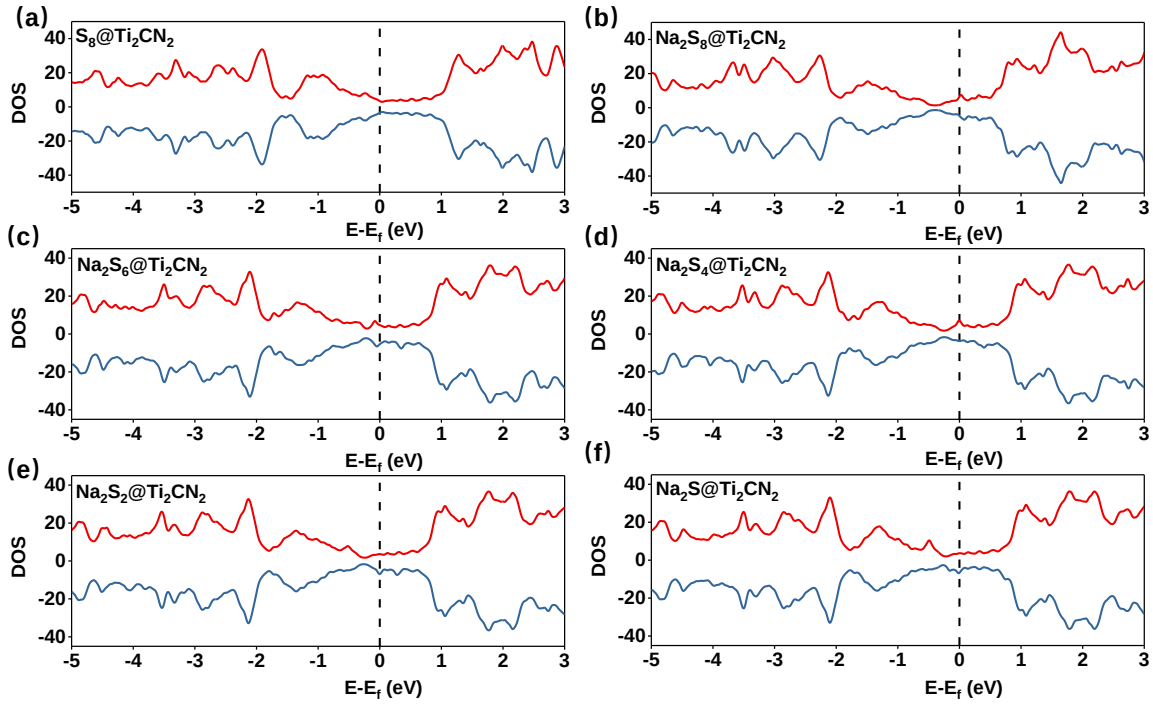

Figure S9. Total density of states (TDOS) of S_8 (a), Na_2S_8 (b), Na_2S_6 (c), Na_2S_4 (d), Na_2S_2 (e), and Na_2S (f) adsorbed on Ti_2CN_2.

References

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