Electronic Supplementary Material (ESI)

Synergistically Boosting the Anchoring Effect and Catalytic Activity of MXenes as Bifunctional Electrocatalysts for Na-S Batteries by Single-Atom Catalysts Engineering

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Table S1 Adsorption energy (eV) of single Fe, Co, Ni, and Cu atom on different sites of Ti_2CS_2

	Fe	Co	Ni	Cu
Type I	- 4.90	- 5.07	- 4.97	- 3.46
Type II	- 4.77	- 5.00	- 4.94	- 3.61

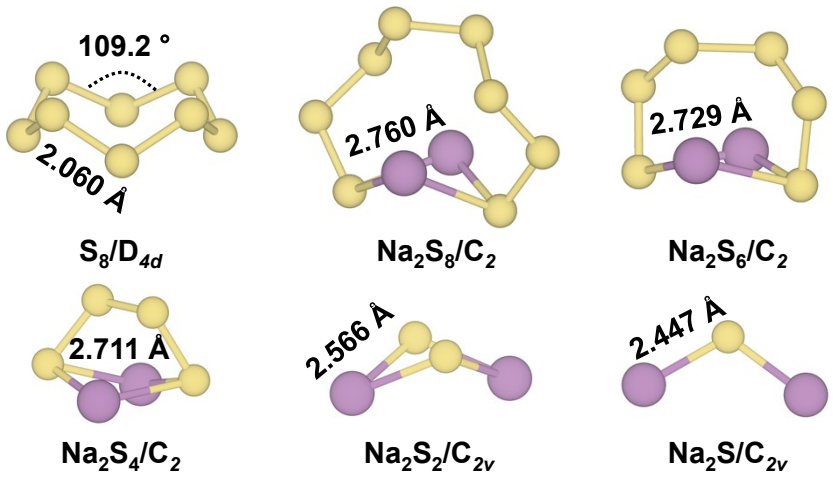
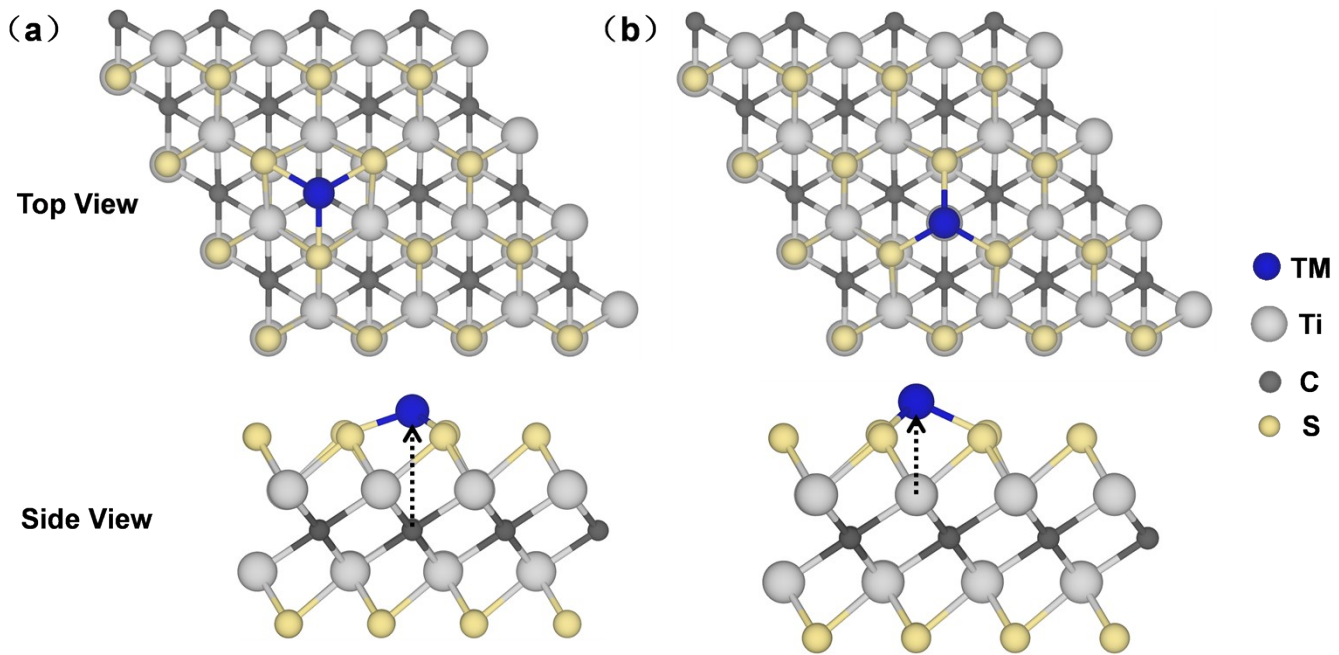


Figure S1. The optimized geometric configurations of S_8 and Na_2S_x ($1 \leq x \leq 8$) clusters in ground-state.

Figure S2. Schematic diagrams of single TM atom supported on top of carbon (a) and titanium (b) atoms of Ti_2CS_2 in the top and side views.



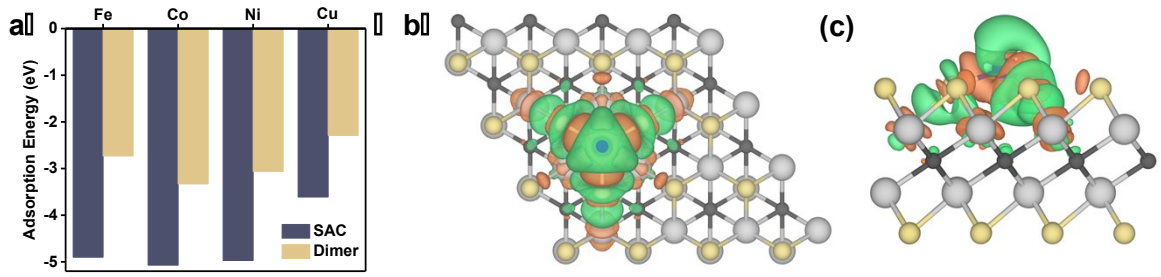


Figure S3. Adsorption energies of single Fe, Co, Ni, and Cu atom immobilized on the surface of Ti_2CS_2 and combined with another TM atom forming corresponding TM dimer (a). Charge density difference of single Fe atom adsorbed on the surface of Ti_2CS_2 substrate in top (b) and side (c) views. Green and orange colors describe electron depletion and accumulation, respectively; The iso-surface level is set to be 0.01 e /Å^3.

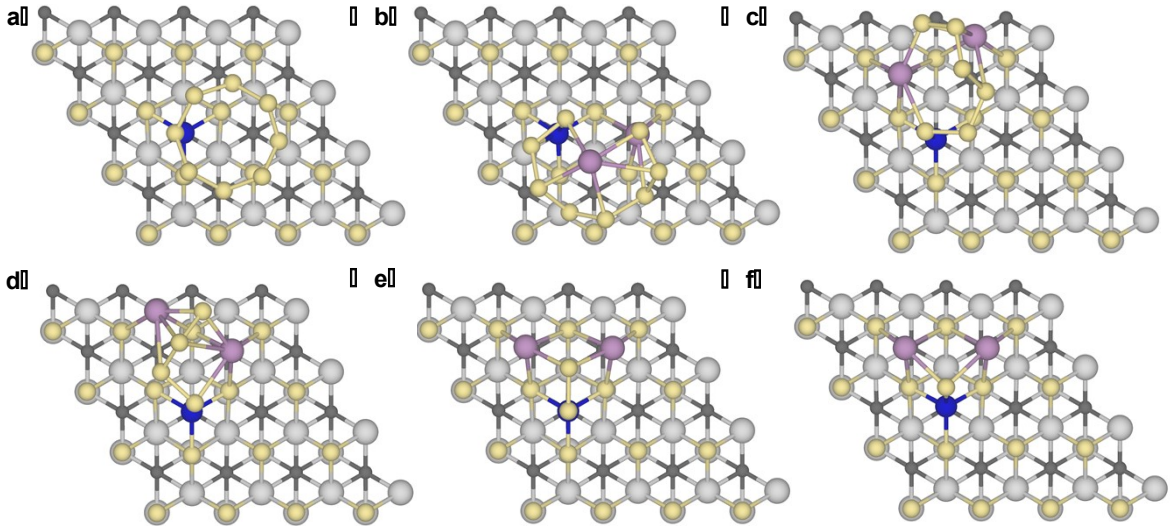


Figure S4. Ground-state configurations of S_8 (a), Na_2S_8 (b), Na_2S_6 (c), Na_2S_4 (d), Na_2S_2 (e), and Na_2S (f) adsorbed on the surface of Fe@Ti_2CS_2 in top view.

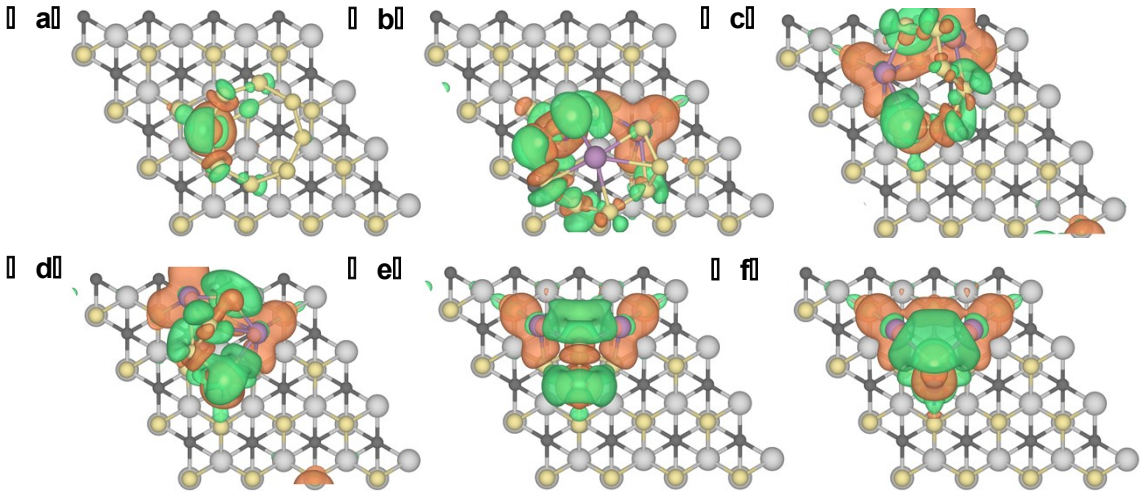


Figure S5. Charge density difference of S_8 (a), Na_2S_8 (b), Na_2S_6 (c), Na_2S_4 (d), Na_2S_2 (e), and Na_2S (f) adsorbed on the surface of Ti_2CS_2 substrate in top view. The iso-surface level is set to be 0.01 e/Å^3. Green and orange colors describe electron depletion and accumulation, respectively.

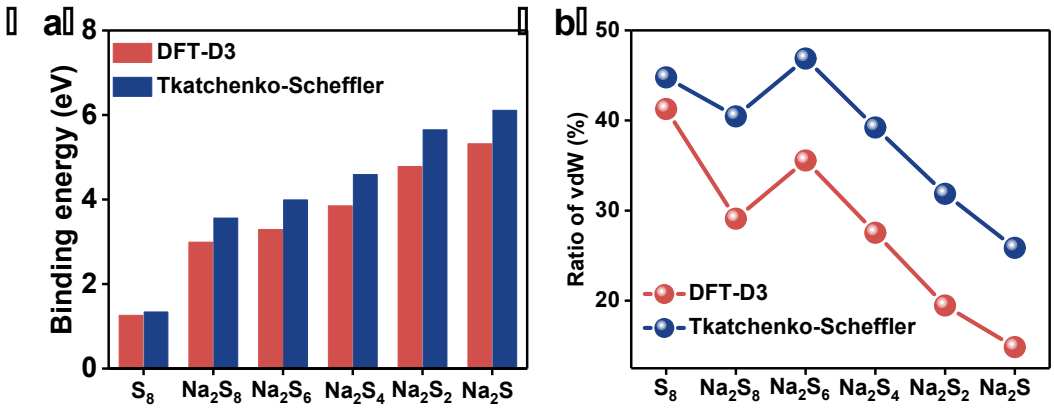


Figure S6. Binding energies (a) and ratio of vdW (b) of various NaPSs on Fe@Ti_2CS_2 by using DFT-D3 and Tkatchenko-Scheffler methods, respectively.

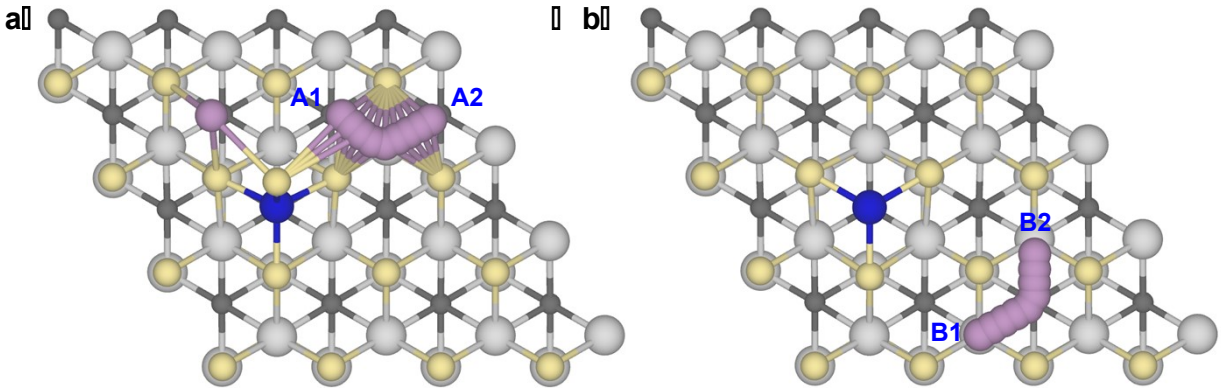


Figure S7. Decomposition path of Na_2S (a), and diffusion path of single Na atom (b) on the surface of $Fe@Ti_2CS_2$.

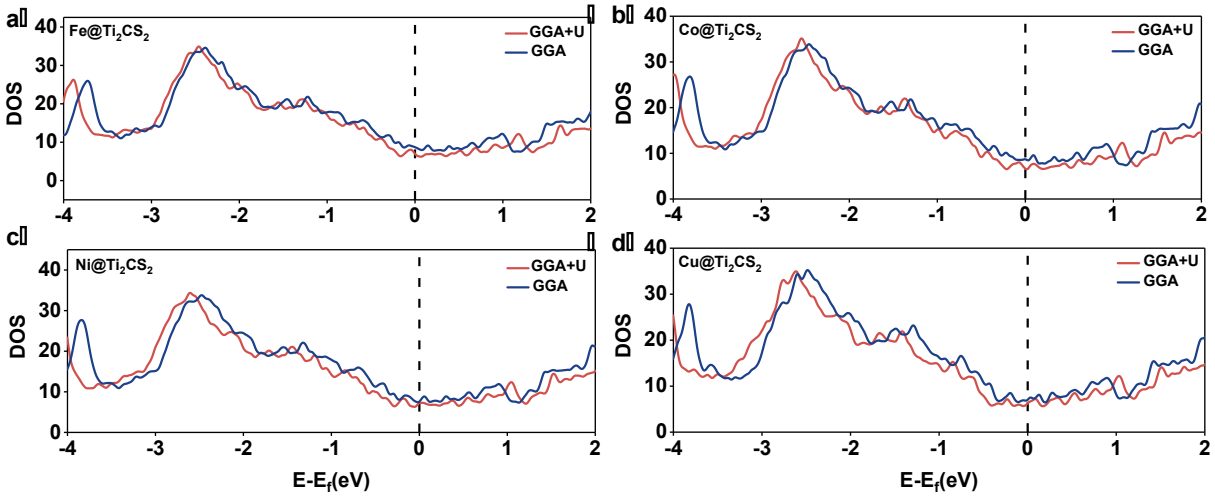


Figure S8. Comparation of total density of states of $TM@Ti_2CS_2$ (TM=Fe, Co, Ni, and Cu) calculated by GGA and GGA+U methods, respectively.

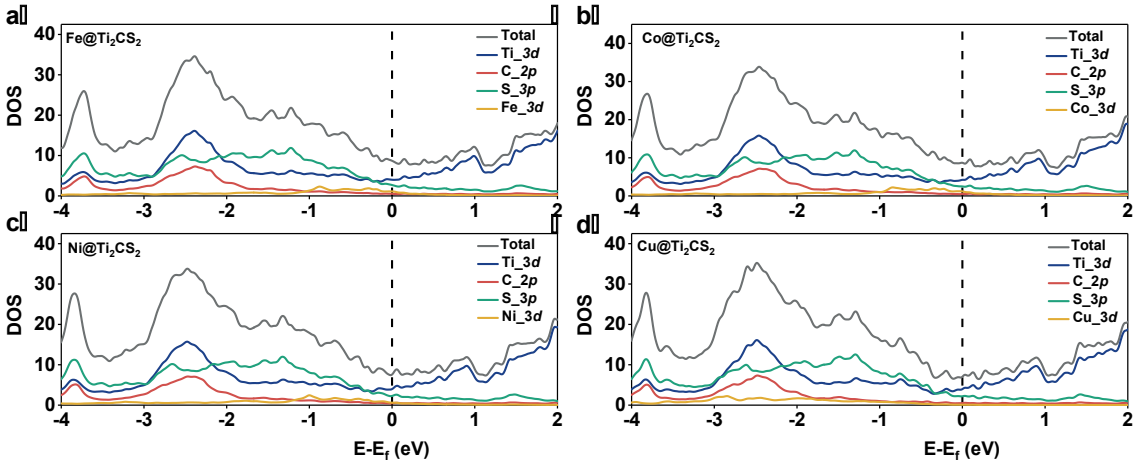


Figure S9. Density of states of TM@Ti_2CS_2 (TM=Fe, Co, Ni, and Cu).

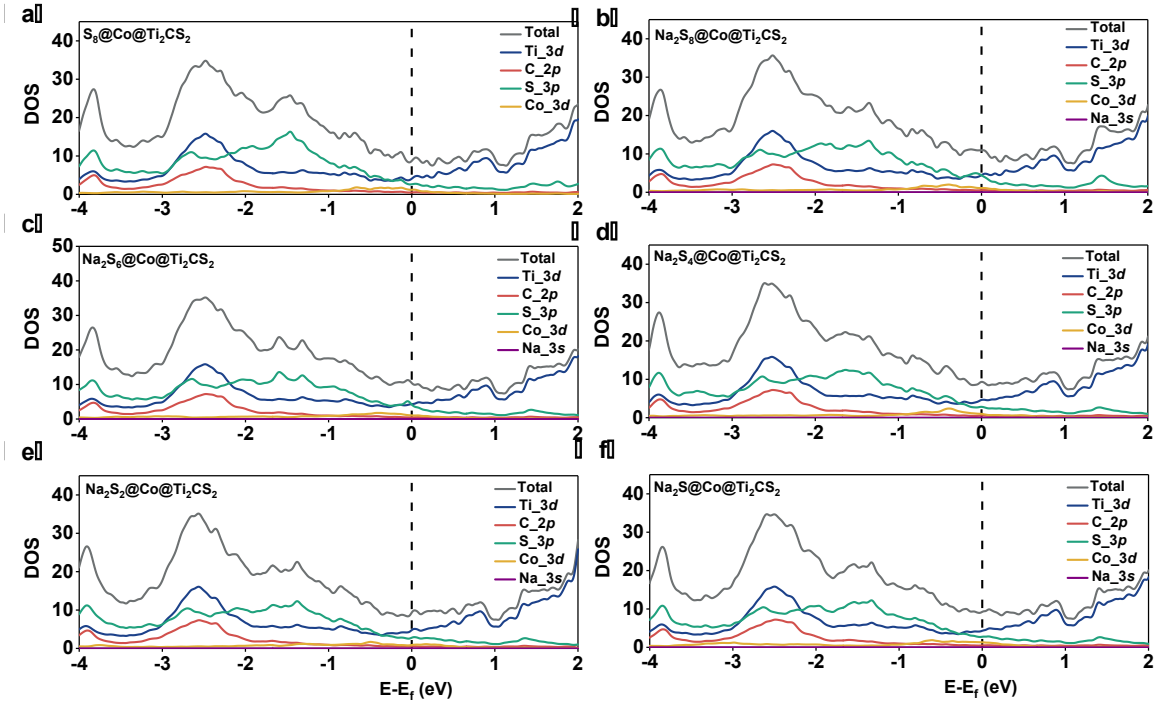


Figure S10. Density of states of S_8 (a), Na_2S_8 (b), Na_2S_6 (c), Na_2S_4 (d), Na_2S_2 (e), and Na_2S (f) adsorbed on the surface of Co@Ti_2CS_2.

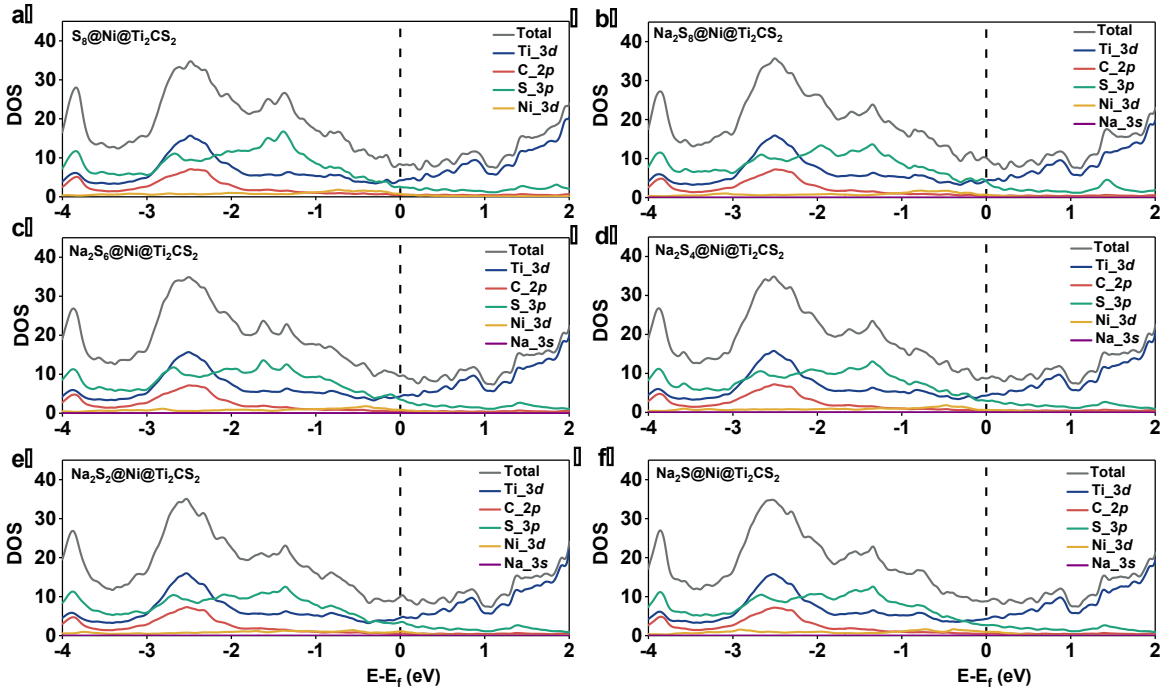


Figure S11. Density of states of S_8 (a), Na_2S_8 (b), Na_2S_6 (c), Na_2S_4 (d), Na_2S_2 (e), and Na_2S (f) adsorbed on the surface of $Ni@Ti_2CS_2$.

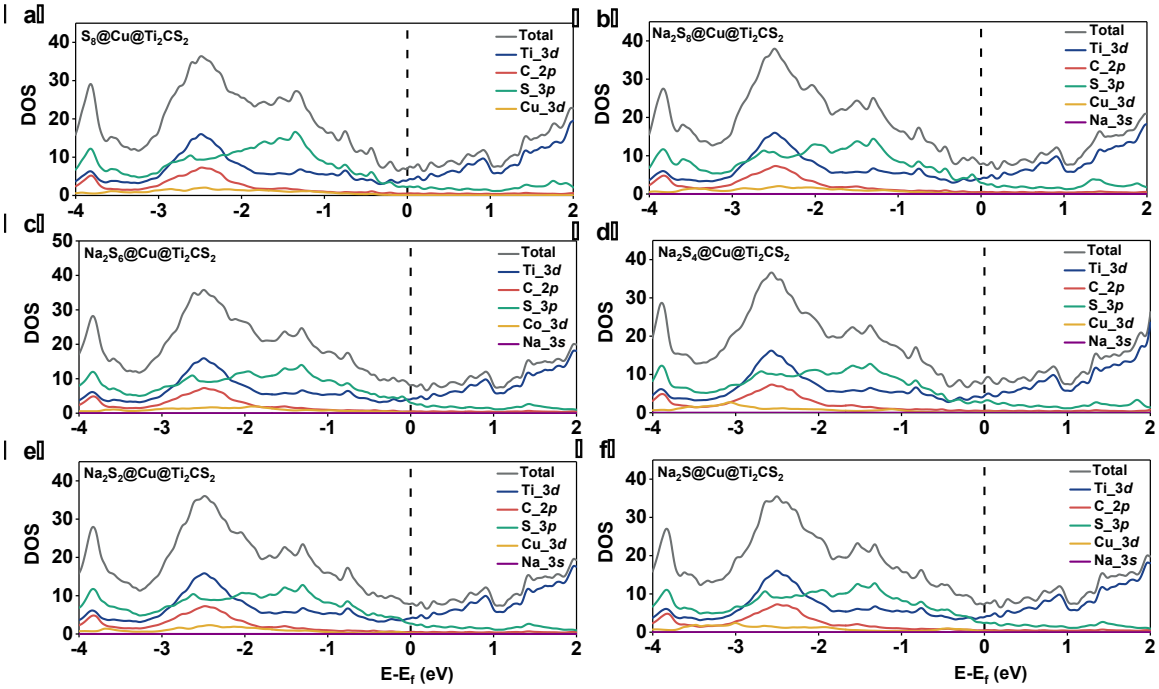


Figure S12. Density of states of S_8 (a), Na_2S_8 (b), Na_2S_6 (c), Na_2S_4 (d), Na_2S_2 (e), and Na_2S (f) adsorbed on the surface of $Cu@Ti_2CS_2$.