Supplementary document

Of

Tuning Polysulfide Adsorption and Catalytic Activity via Surface Functionalization of Nb_2TiN_2 MXene in Na–S Batteries

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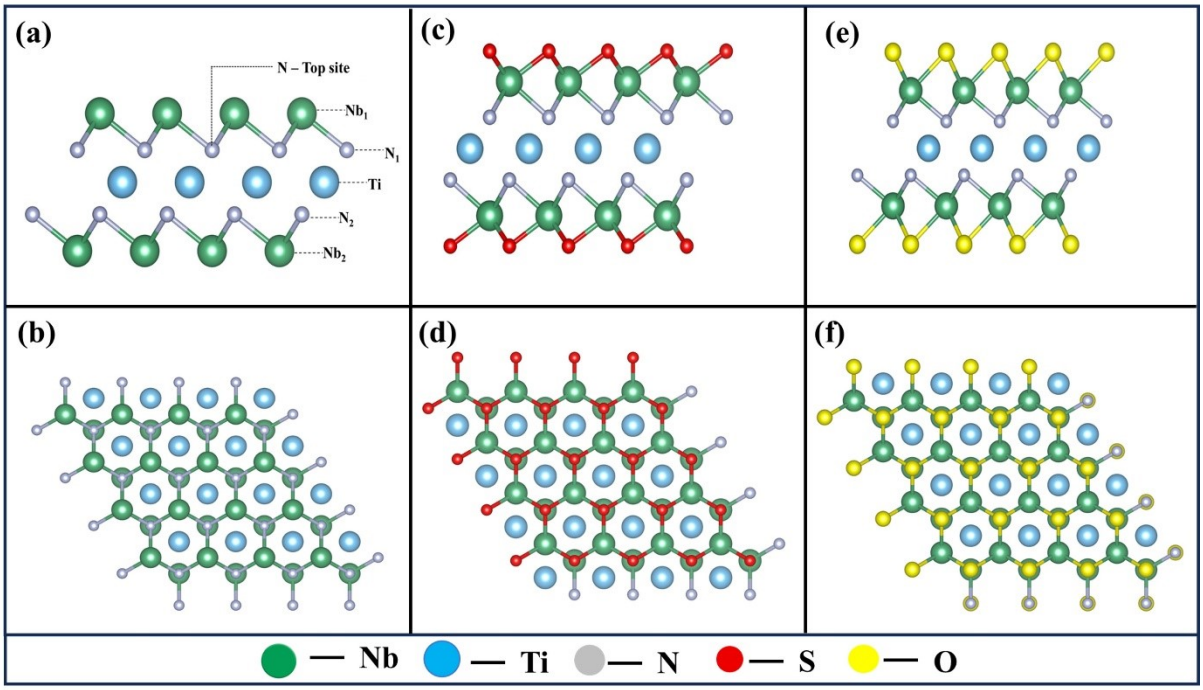

Figure S1: Optimized geometric configurations of Pristine and surface functionalized DTM-MXene. (a) side view of pristine Nb_2TiN_2 showing N – Top site is a preferred termination site. (b) Top view of pristine Nb_2TiN_2. (c) and (d): Side and Top views of $Nb_2TiN_2O_2$, respectively. (e) and (f): Side and Top views of $Nb_2TiN_2S_2$, respectively.

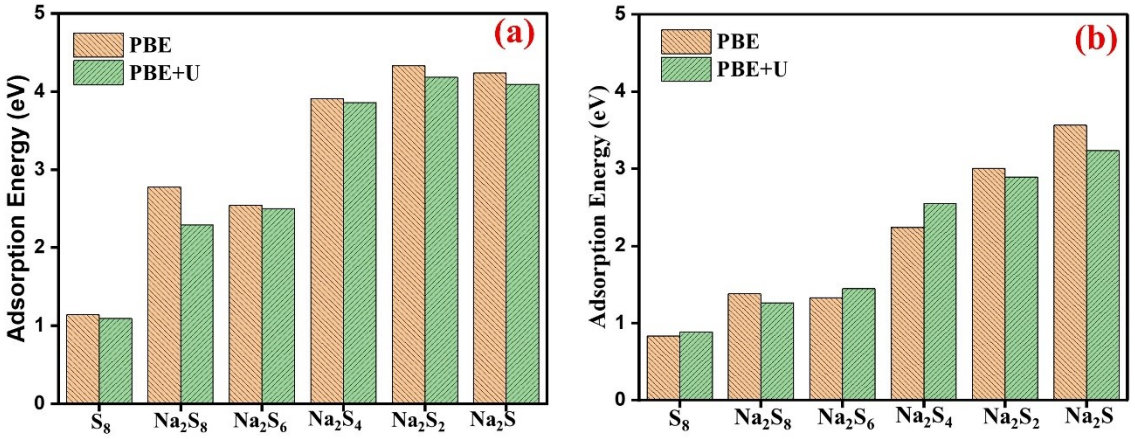

Figure S2: The adsorption energies of S_8 and Na_2S_n (n = 2,4,6,8) adsorbed on (a). $Nb_2TiN_2O_2$ (b). $Nb_2TiN_2S_2$ are calculated by employing the PBE and PBE+U methods, respectively.

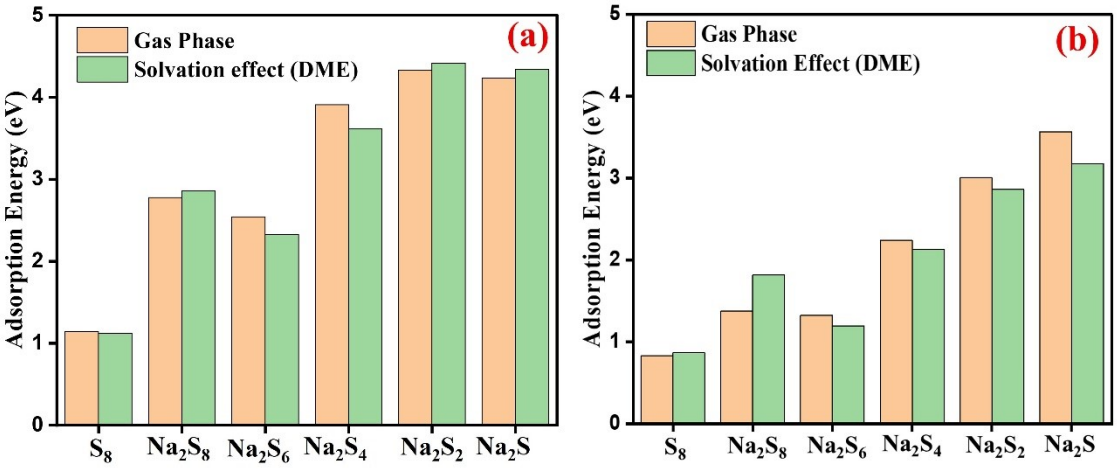

Figure S3. The adsorption energies of S_8 and Na_2S_n (n = 2,4,6,8) adsorbed on (a). $Nb_2TiN_2O_2$ (b). $Nb_2TiN_2S_2$ are calculated by employing gas phase and implicit solvation model, respectively.