Supplementary Information (SI) for Physical Chemistry Chemical Physics.

Uniaxial Tensile Strain effect on 1T-NbS_2 Monolayers as a Potential Cathode Material for Lithium-Sulfur Batteries

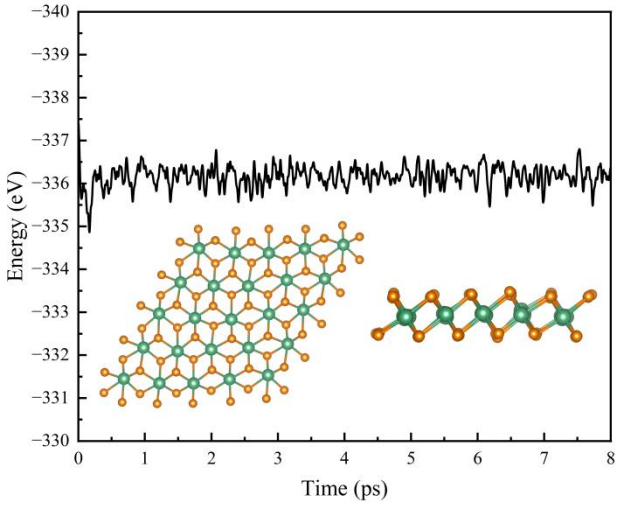

Fig S1. AIMD simulations of the strained 1T-NbS_2 monolayers for 8 ps under 300K. The insets are the top and side views of the final structure.

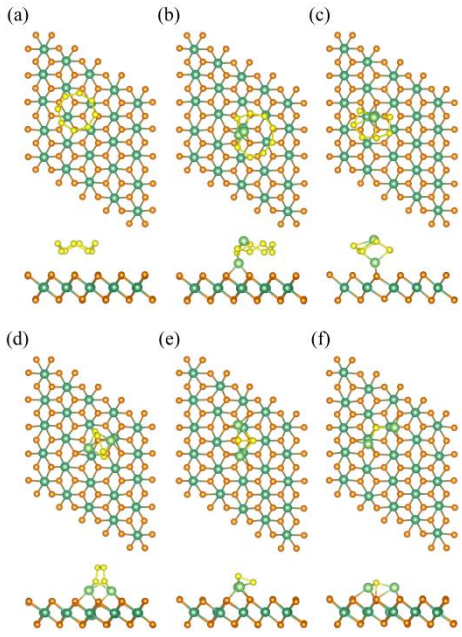

Fig S2. The panels (a) to (f) show the most stable adsorption configurations of S_8/Li_2S_n on the pristine 1T-NbS_2 monolayer surface, corresponding to n = 8, 6, 4, 2, and 1 respectively. In these figures, orange and dark green spheres represent S and Nb atoms in the 1T-NbS2 monolayer while yellow and light green spheres represent S and Li atoms in S_8/Li_2S_n.

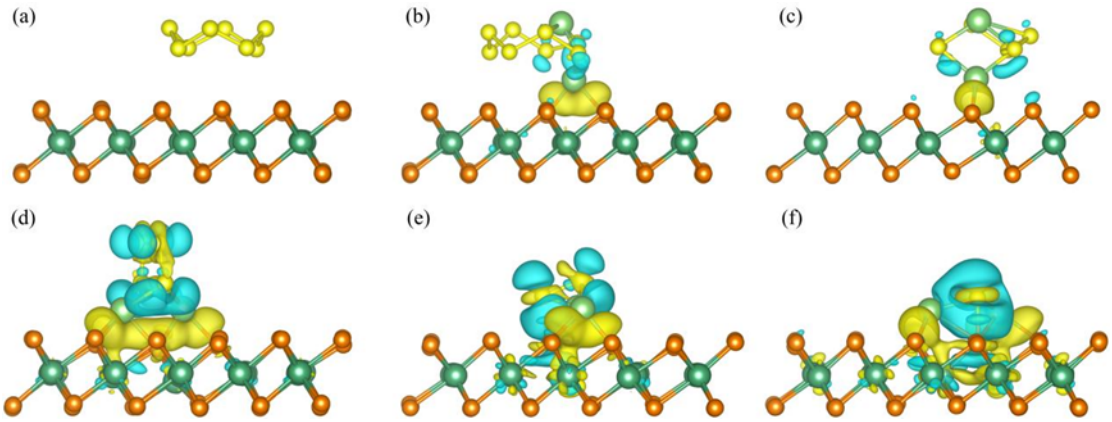

Fig S3. The charge density of S_8/Li_2S_n clusters on the pristine 1T-NbS_2 monolayer changes. (a) to (f) represent S_8 and Li_2S_n (n= 8,6,4,2,1), respectively. Yellow areas indicate charge accumulation while blue areas indicate charge depletion. The isosurface threshold is set at 0.002e/A³.

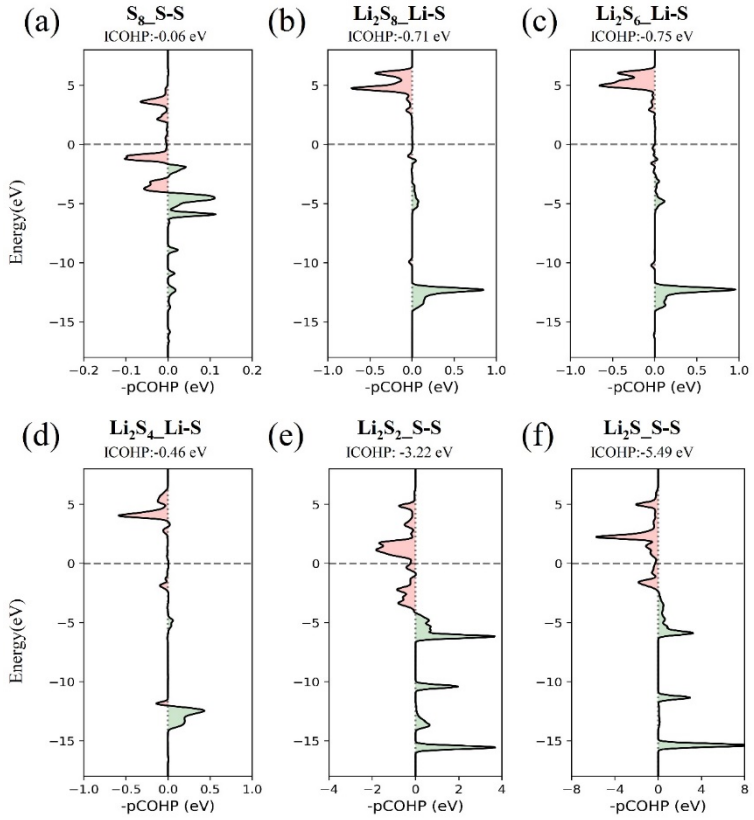

Fig S4. (a) ~ (f) COHP diagram of the shortest two atoms between S_8/Li_2S_n (n=8,6,4,2,1) and the pristine 1T-NbS_2 monolayer surface. The bonding states are depicted in green, and the antibonding states are in red.

		S_8	Li_2S_8	Li_2S_6	Li_2S_4	Li_2S_2	Li_2S
Pristine	d_{min} (Å)	3.49906	2.48177	2.45467	2.46000	2.25796	2.07258
Post strain	d_{min} (Å)	3.53448	2.45963	2.49937	2.41671	2.23797	2.06947

Table S1. The shortest atom distance (d_{min}) between S_8/Li_2S_n (n= 8, 6, 4, 2, 1) cluster and substrate on the surface of the pristine and strained 1T-NbS_2 monolayer.

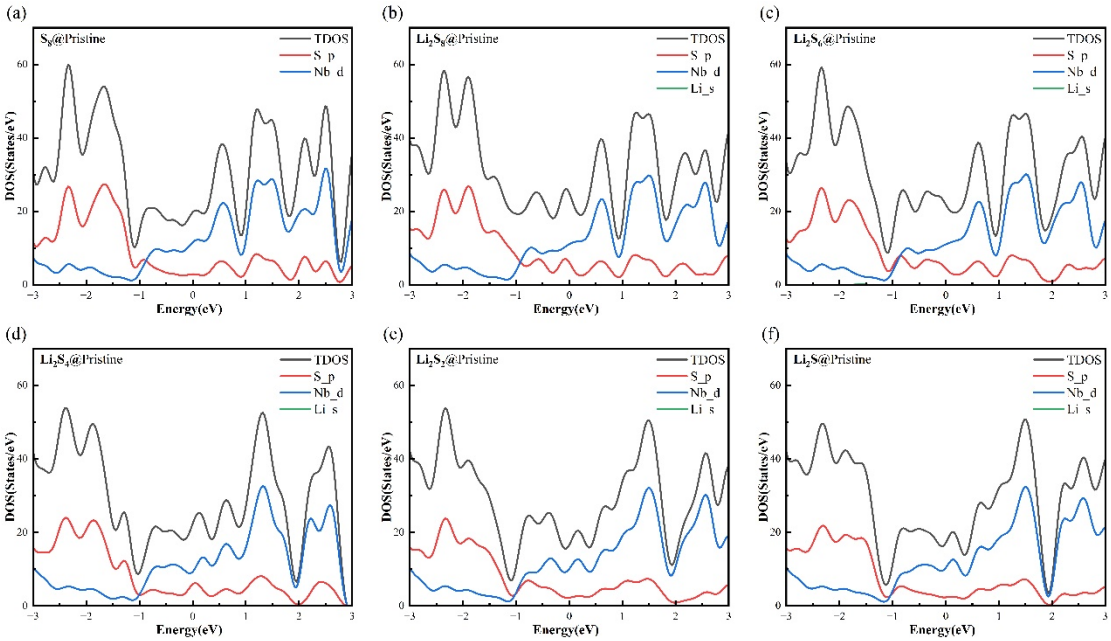

Fig S5. (a) ~ (f) The projected density of states(PDOS) of S_8/Li_2S_n (n= 8, 6, 4, 2, 1) adsorbed to the pristine 1T-NbS2 monolayer surface.

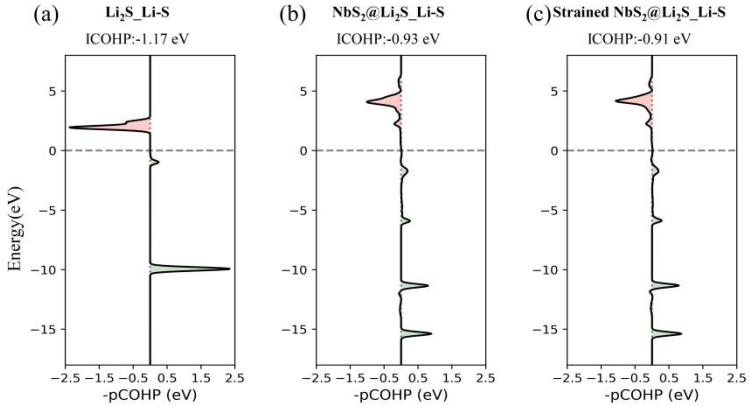

Fig S6. (a) ~ (c) COHP diagram of isolated Li_2S, Li_2S adsorbed on the pristine 1T-NbS_2 monolayer surface and the strained 1T-NbS_2 monolayer surface. The bonding states are depicted in green, and the antibonding states are in red.