Supporting Information

DFT Simulation-Based Design of 1T-MoS_2 Cathode Hosts for Li-S Batteries and Experimental Evaluation

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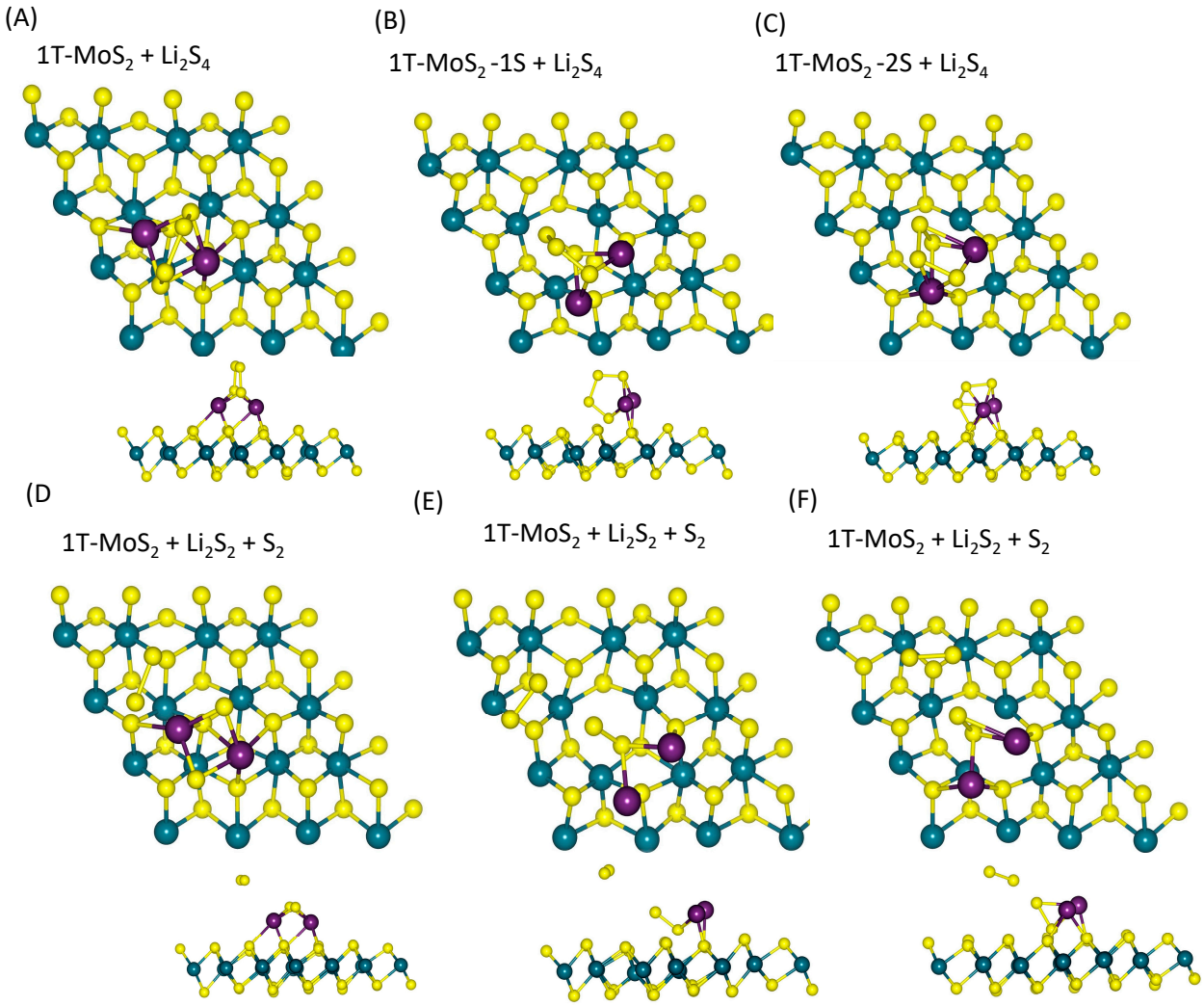

Figure S1. Top views and side views of the optimised geometry of adsorbed Li_2S_4 on (A) 1T-MoS_2, (B) 1T-MoS_2-1S, (C) 1T-MoS_2-2S; (D), (E), (F) its dissociated products on 1T-MoS_2, 1T-MoS_2-1S, 1T-MoS_2-2S, respectively for the reaction pathway of $Li_2S_4 \rightarrow Li_2S_2 + S_2$. The S-S bond length was less than 5 Å.

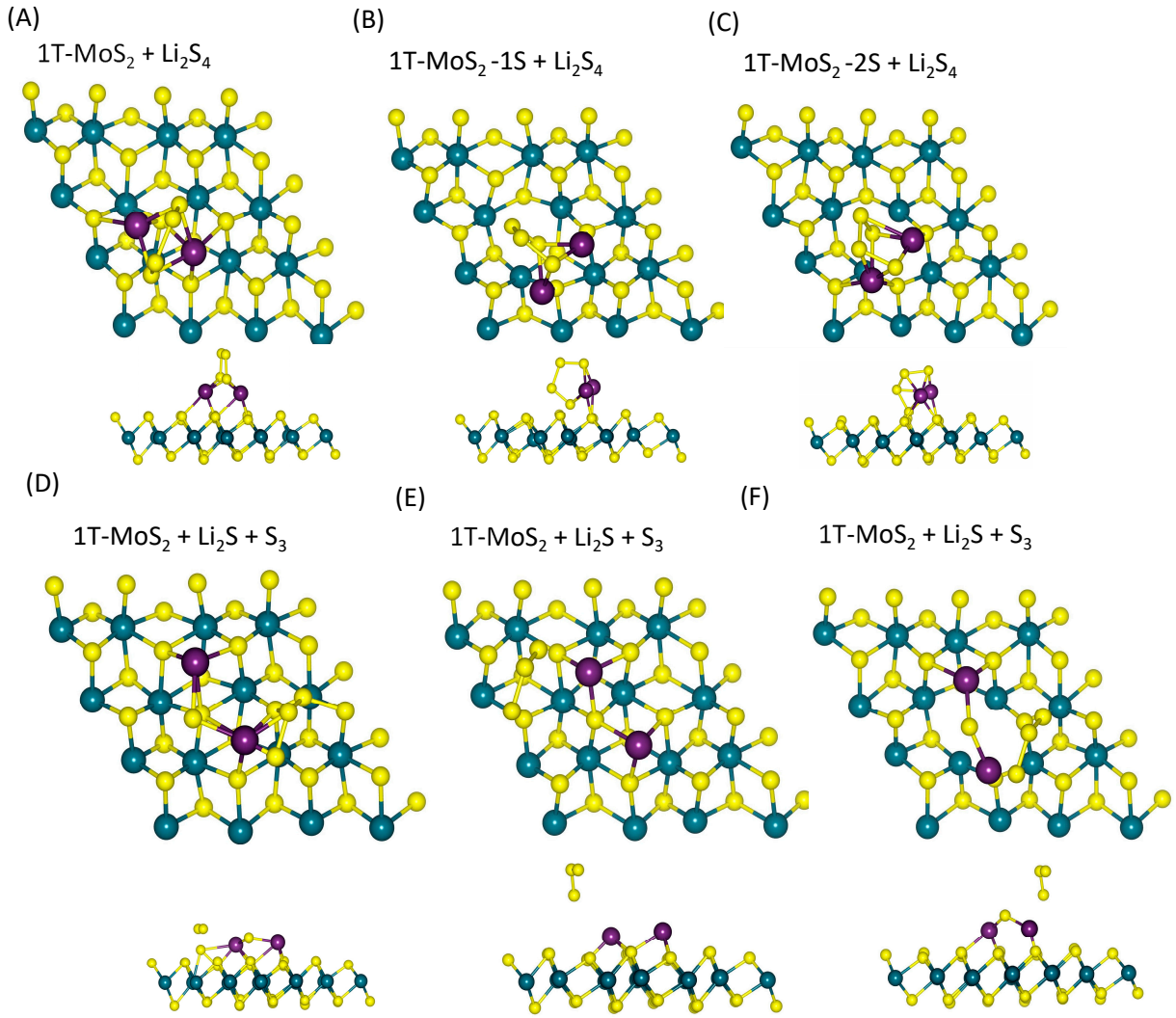

Figure S2. Top views and side views of the optimised geometry of adsorbed Li_2S_4 on (A) 1T-MoS_2, (B) 1T-MoS_2-1S, (C) 1T-MoS_2-2S; (D), (E), (F) its dissociated products on 1T-MoS_2, 1T-MoS_2-1S, 1T-MoS_2-2S, respectively for the reaction pathway of $Li_2S_4 \rightarrow Li_2S + S_3$. The S-S bond length was less than 5 Å.