Supporting Information

Asymmetric Ti_2CO/WS_2 heterostructure as a promising anchoring material for lithium-sulfur batteries

Qin Fang, †[a] Min Fang, †[a] Xinyi Liu,[a] Pengfei Yu,[a] Ji-Chang Ren,[a] Shuang Li*[a] and Wei Liu*[a]

[a]Nano and Heterogeneous Materials Center, School of Materials Science and Engineering,

Nanjing University of Science and Technology, Nanjing 210094, China

† Both authors contributed equally to this work.

Corresponding authors: lishuang@njust.edu.cn; weiliu@njust.edu.cn

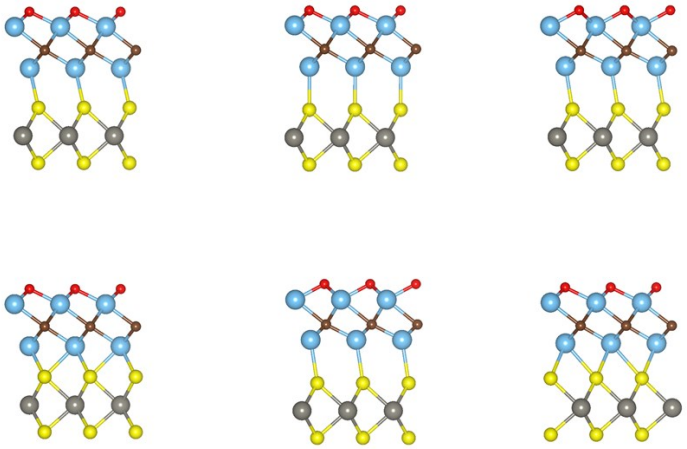

Fig. S1. The considered stacking patterns for the Ti_2CO/WS_2 bilayer. The red, blue, brown, yellow and gray balls represent the oxygen, titanium, carbon, sulfur and tungsten atom respectively.

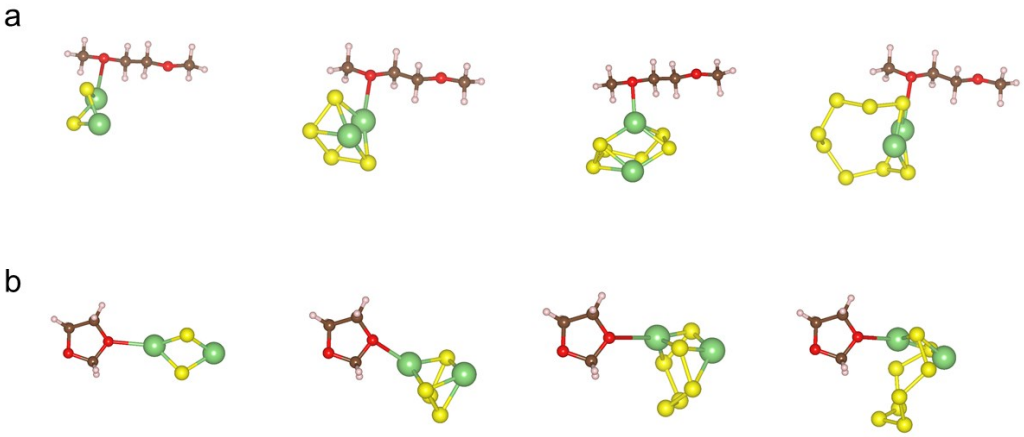

Fig. S2. Configurations of Li_2S_n (n=2,4,6,8) bound with (a) DME and (b) DOL. The red, brown, white, yellow and green balls represent the oxygen, carbon, hydrogen, sulfur and lithium atom respectively.

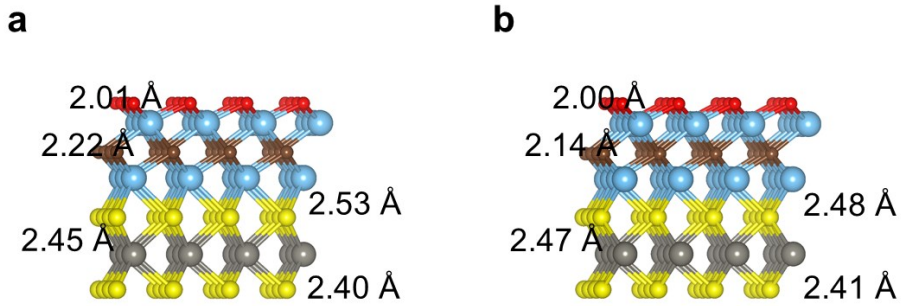

Fig. S3. The side views of the Ti_2CO/WS_2 structure (a) before and (b) after AIMD runs for 5 ps. All atoms are displacing slightly near their equilibrium positions during the simulations and no structural reconstruction occurs at 298 K.

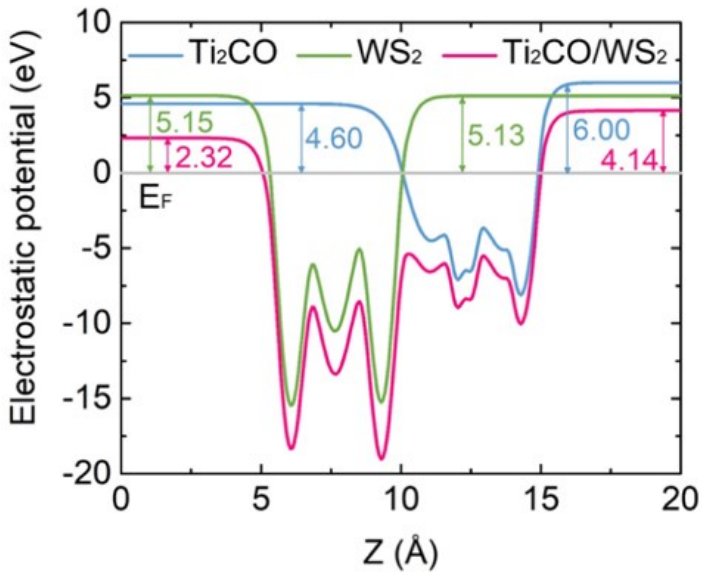

Fig. S4. The plane-averaged electrostatic potential of Ti_2CO, WS_2 before contacting and Ti_2CO/WS_2 after contacting.

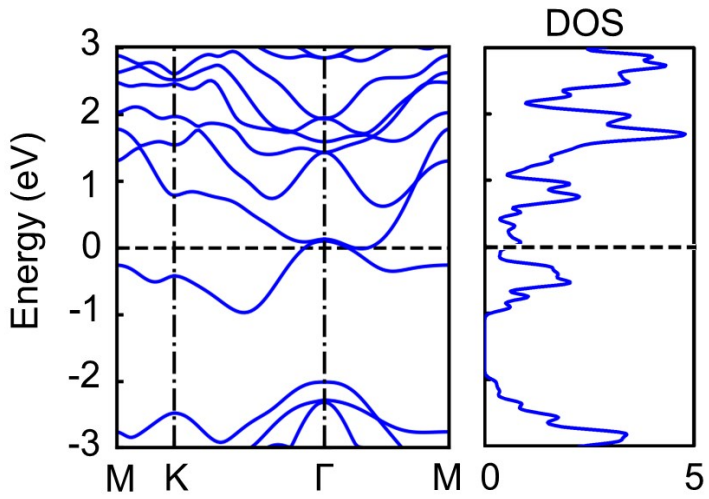

Fig. S5. The band structure and total electron density of states for Ti_2CO/WS_2 heterostructure by using HSE06 method.

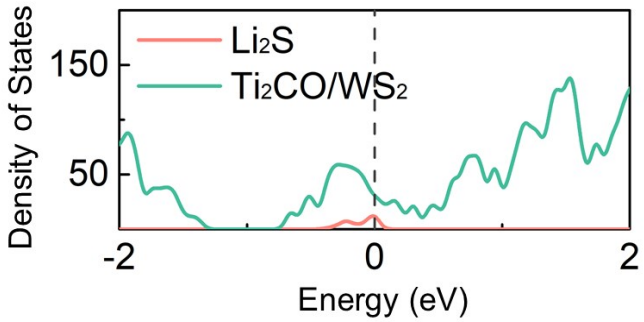

Fig. S6. The projected DOS of Li_2S and Ti_2CO/WS_2 in Li_2S-Ti_2CO/WS_2 system.