Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

Supporting information

Borophene and defective borophene as the potential anchoring materials for lithium-sulfur batteries: a first-principles study

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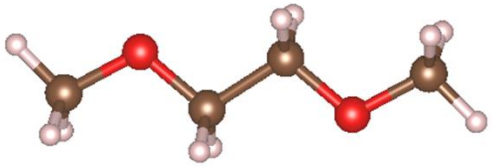

Fig. S1. The optimized structures of DME. The brown, red and white balls represent for carbon, oxygen and hydrogen, respectively.

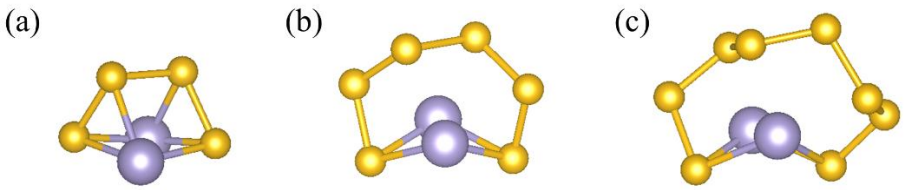

Fig. S2. The most stable structures of (a) Li_2S_4, (b) Li_2S_6 and (c) Li_2S_8. The yellow and purple balls represent for sulfur and lithium, respectively.

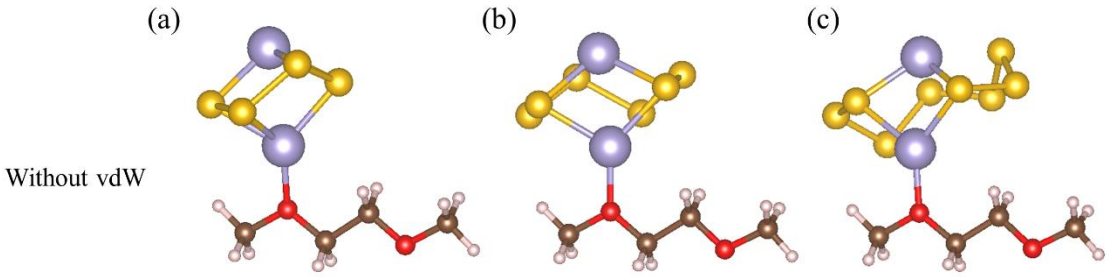

Fig. S3. The most stable structures of (a) Li_2S_4, (b) Li_2S_6 and (c) Li_2S_8 adsorbed on DME simulated without vdW functional.

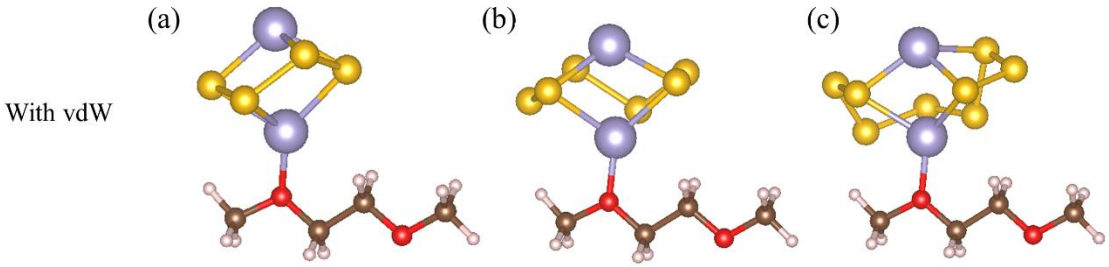

Fig. S4. The most stable structures of (a) Li_2S_4, (b) Li_2S_6 and (c) Li_2S_8 adsorbed on DME simulated with vdW functional.

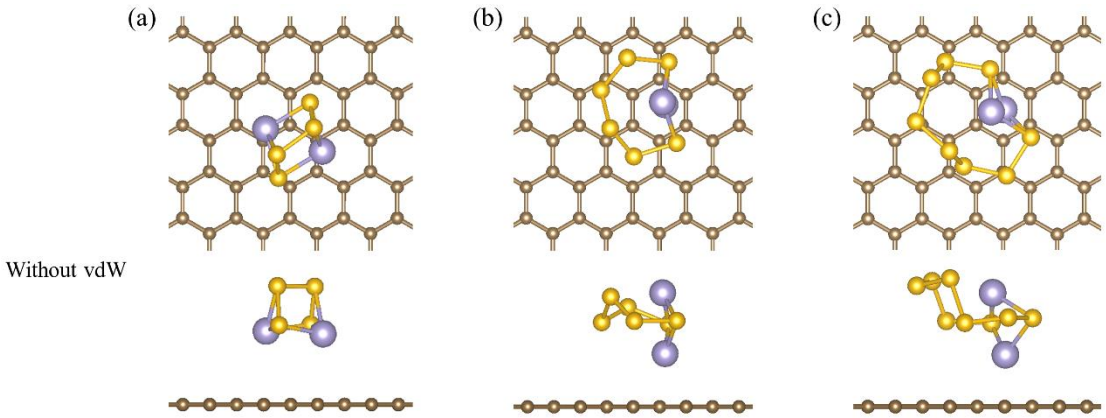

Fig. S5. The most stable structures of (a) Li_2S_4, (b) Li_2S_6 and (c) Li_2S_8 adsorbed graphite (0001) surface simulated without vdW functional.

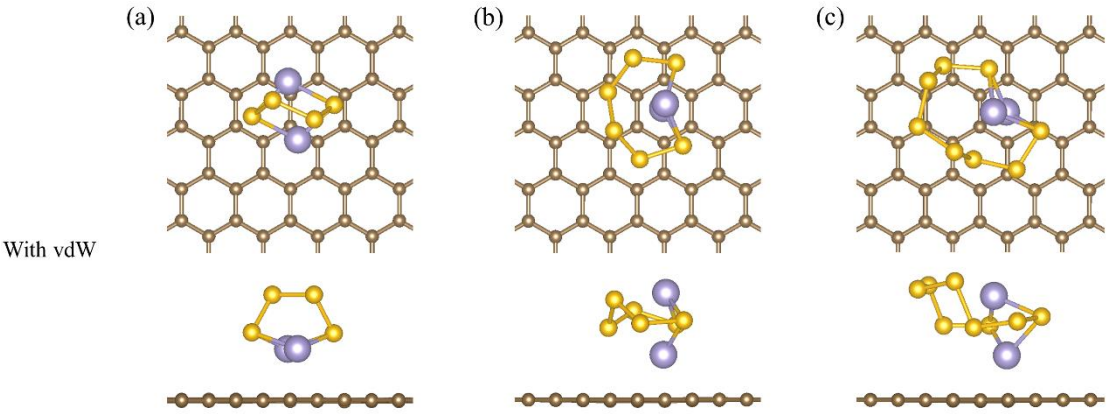

Fig. S6. The most stable structures of (a) Li_2S_4, (b) Li_2S_6 and (c) Li_2S_8 adsorbed graphite (0001) surface simulated with vdW functional.

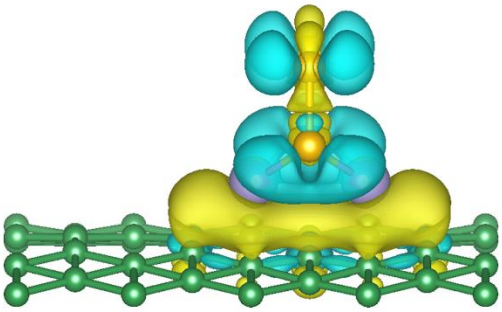

Fig. S7. The charge difference plot of Li_2S_4 on defective borophene. The blue and yellow areas represent for electron loss and gain.

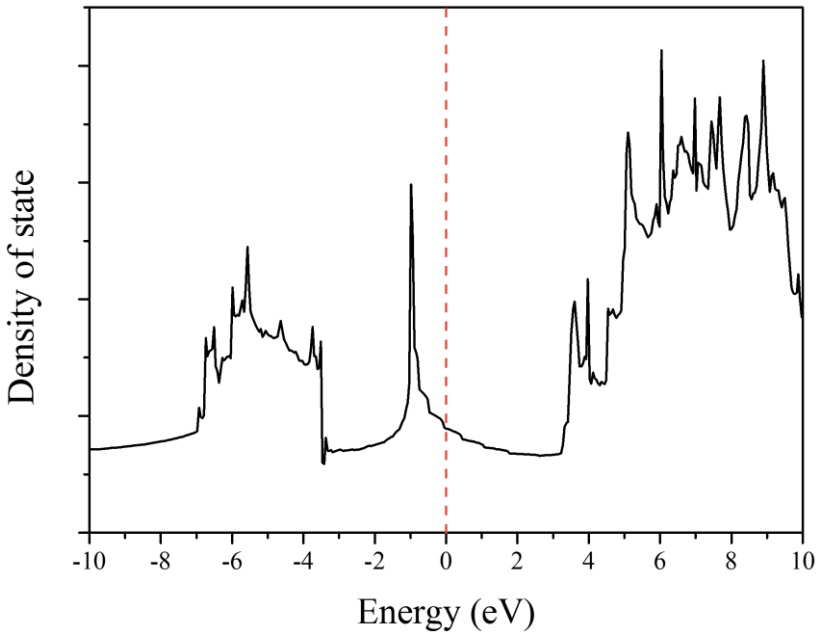

Fig. S8. The DOS of pristine borophene.