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Supplementary Information

For

Understanding the interaction of N-doped graphene and sulfur compounds in a lithium-sulfur battery – a density functional theory investigation

Yingying Gong [a], Wanyong Ma [a], Zhen Xu [*a], Yixuan Wang [*b]

[a]School of Chemistry and Pharmaceutical Engineering, Qilu University of Technology (Shandong Academy of Sciences), Jinan 250010, PR China.

[b]Computational Chemistry Laboratory, Department of Chemistry and Forensic Sciences, Albany State University, Albany, GA31705, USA.

[*]Corresponding author E-mail: xuzhen123@126. com (Dr. Xu)

ywang@asurams.edu (Prof. Wang)

The top view of optimal configurations

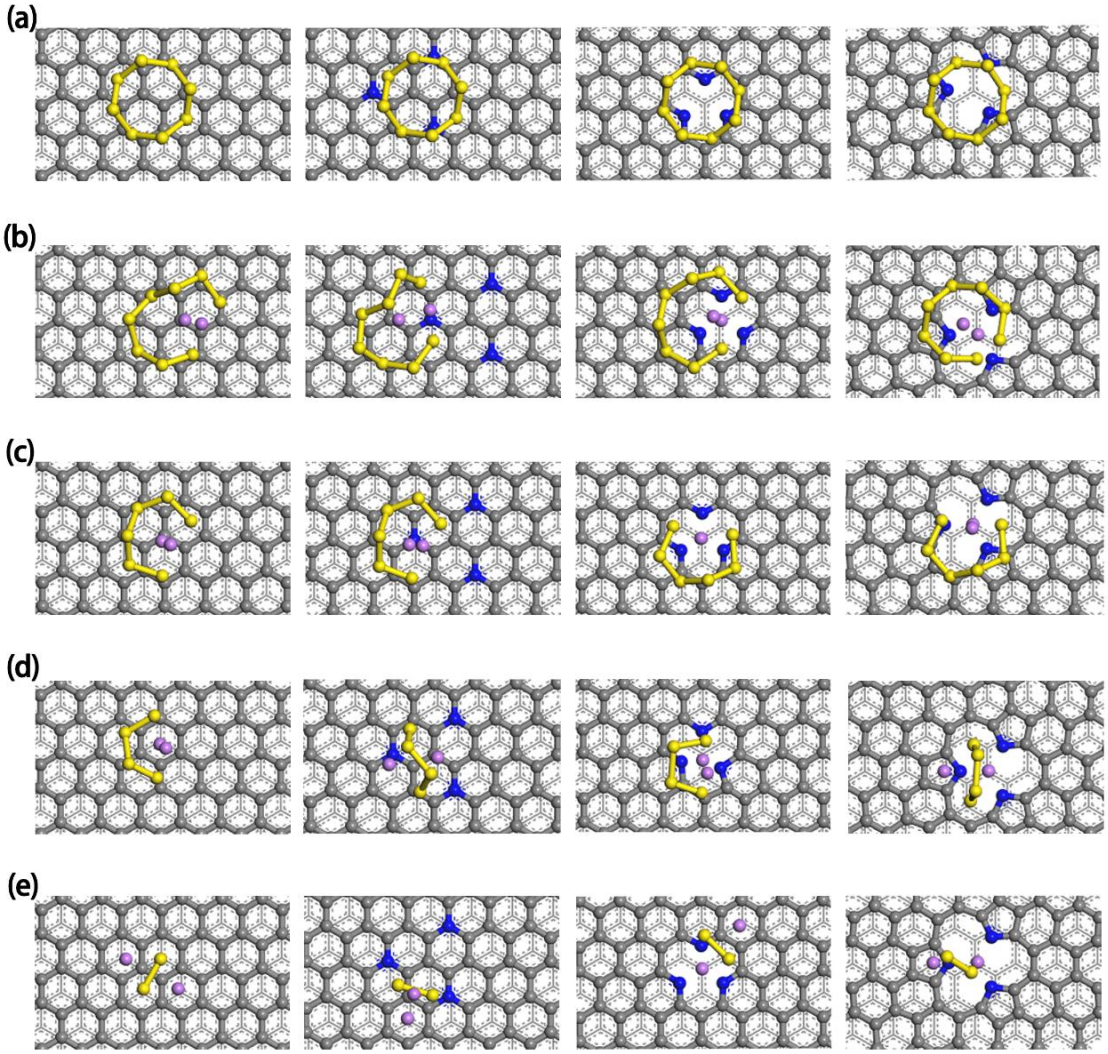

Fig. S1 Top view of after adsorption of (a) S_8 (b) Li_2S_8 (c) Li_2S_6 (d) Li_2S_4 (e) Li_2S_2 with graphene and the content of different nitrogen species, respectively.

The side view of optimal configurations

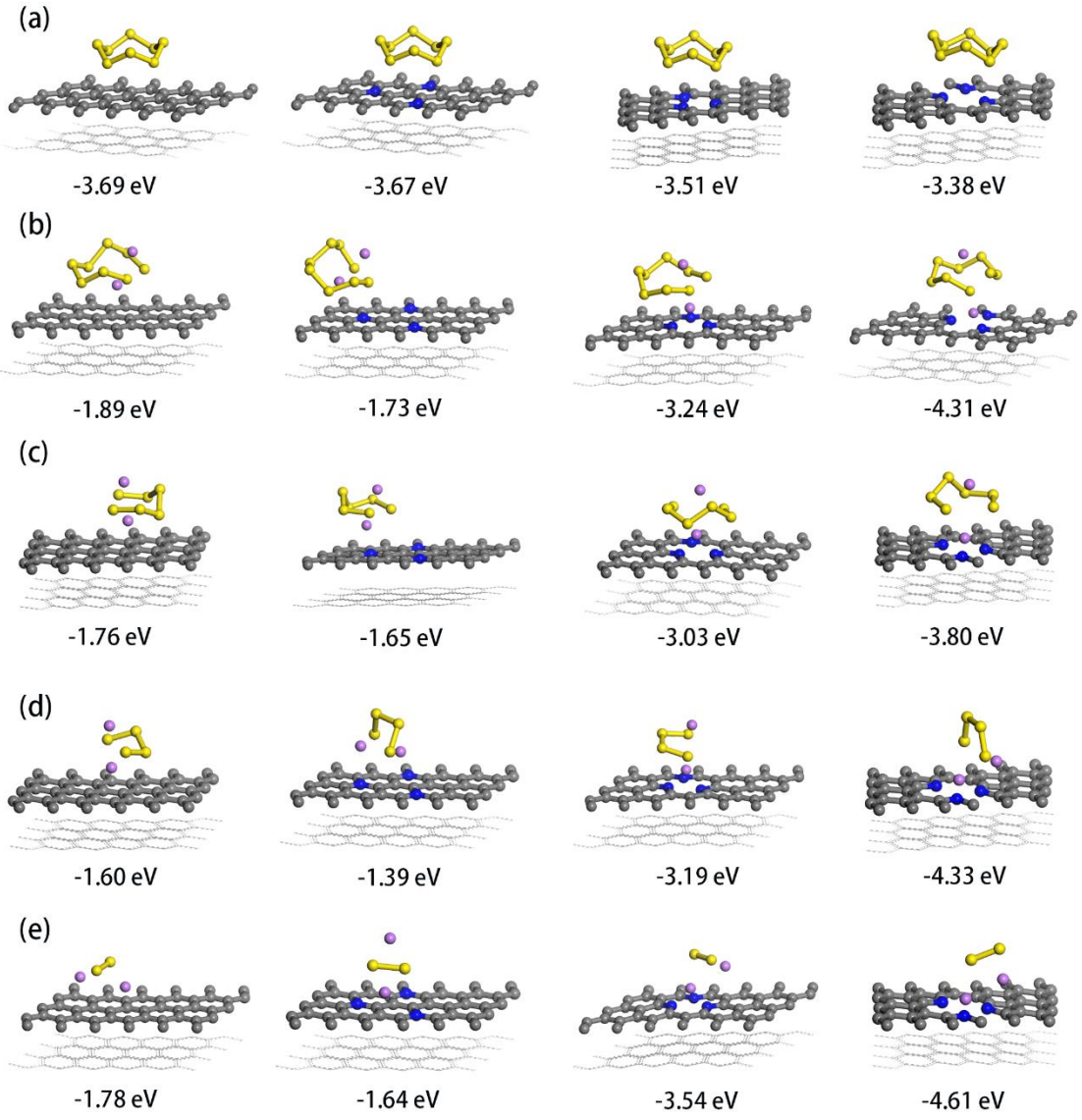

Fig. S2 Side view of after adsorption of (a) S_8 (b) Li_2S_8 (c) Li_2S_6 (d) Li_2S_4 (e) Li_2S_2 with graphene and the content of different nitrogen species, respectively. Note the adsorption value of each configuration is explained below the figures.

The side view of other optimized configurations

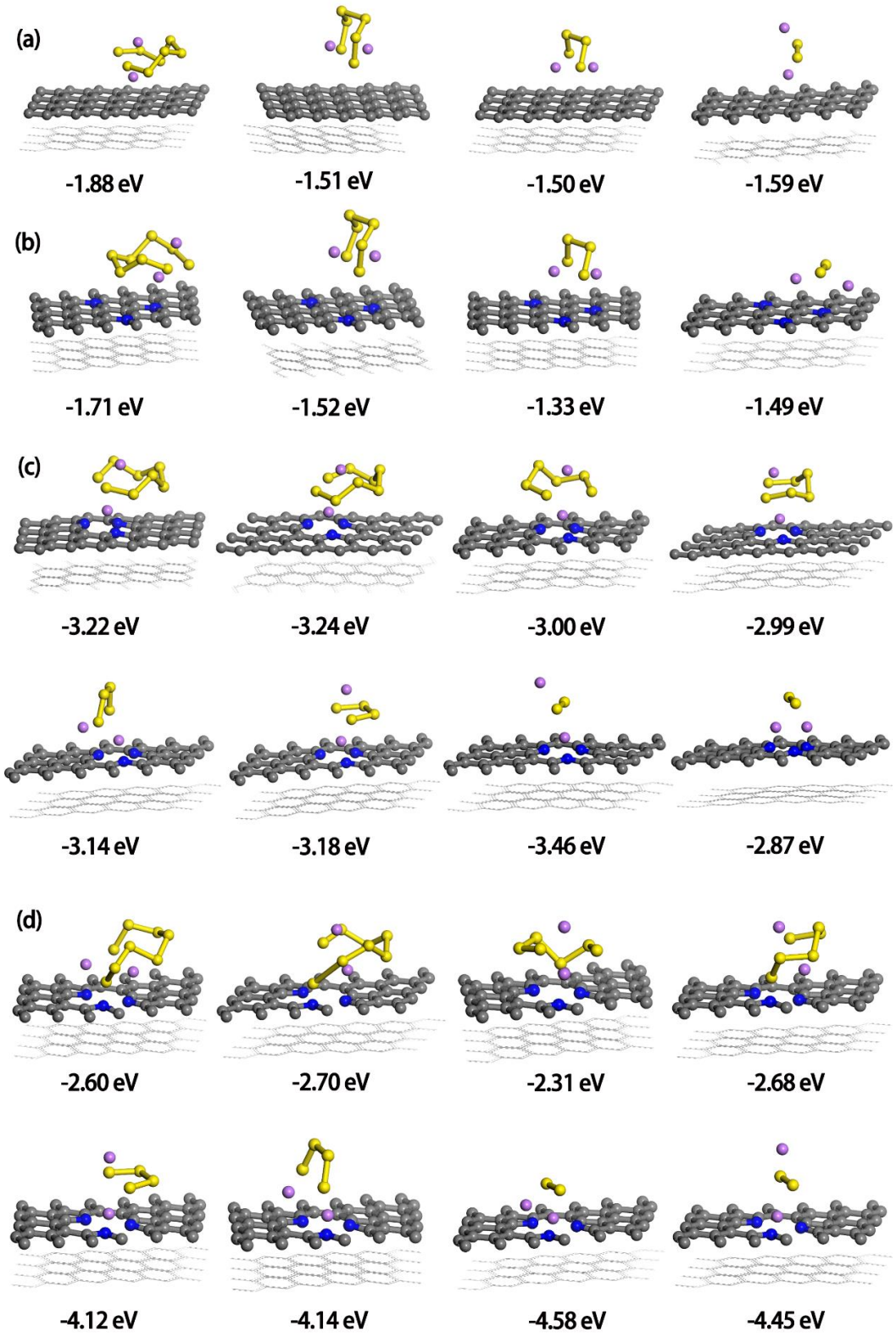

Fig. S3 Different configurations and corresponding adsorption energies of Li_2S_x (x=8,6,4,2) adsorbed on graphene (a), graphitic N(b), pyridinic N (c) and pyrrolic N (d).