Supporting Information for

Understanding the Inhibition of the Shuttle Effect of Sulfides (S ≤ 3) in Lithium-Sulfur Batteries by Heteroatom-Doped Graphene: First-Principles Study

Benjie Gong, Xuedan Song*, Yantao Shi, Jianhui Liu, Ce Hao

State Key Laboratory of Fine Chemicals, School of Chemical Engineering, Dalian University of Technology, Dalian, 116024, China

*E-mail: song@dlut.edu.cn

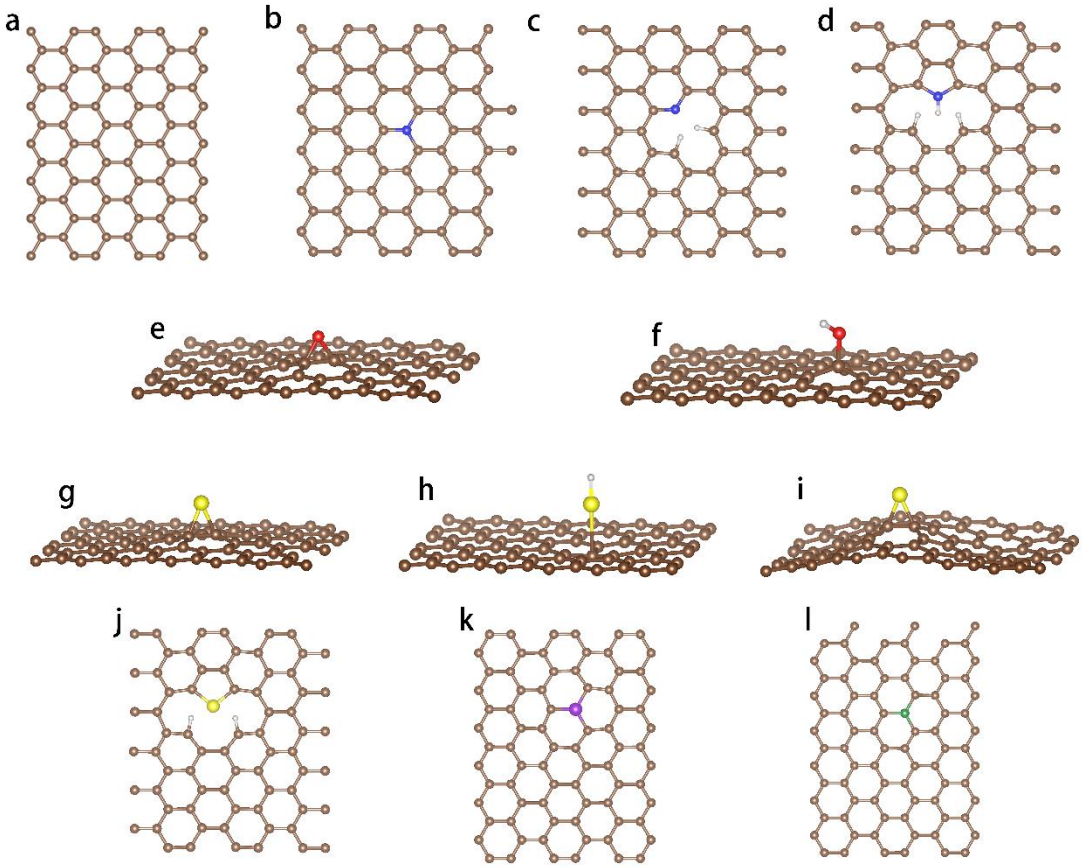

Fig. S1. Optimized configuration of (a) undoped graphene (b) graphitic nitrogen (c) pyridine nitrogen (d) pyrrolic nitrogen (l) graphitic boron (k) phosphorus (e) epoxy group (f) hydroxyl group (g) episulfide group (h) sulfydryl group (i) sulfur defect (j) thiophene sulfur.

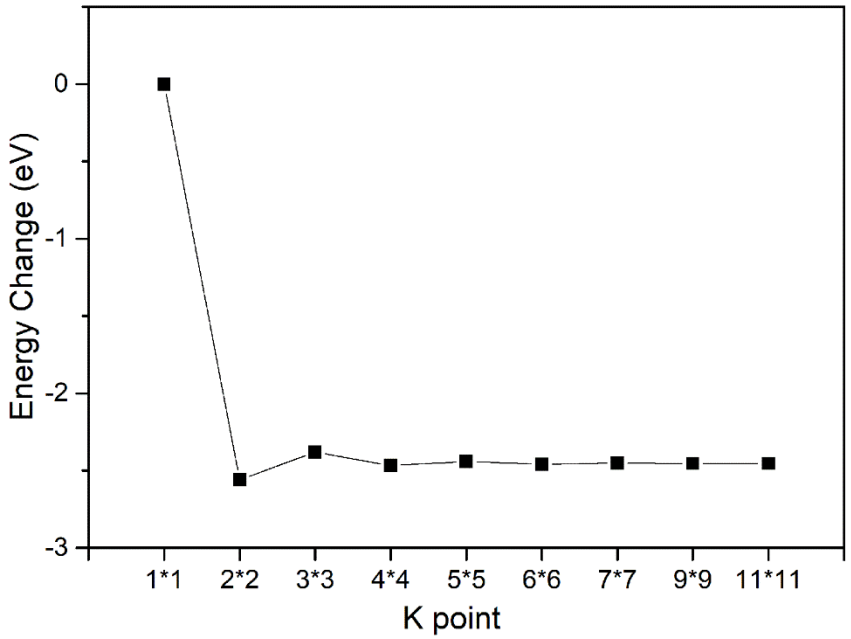

Fig. S2. Convergence test of K point along the periodical direction of perfect graphene sheet.

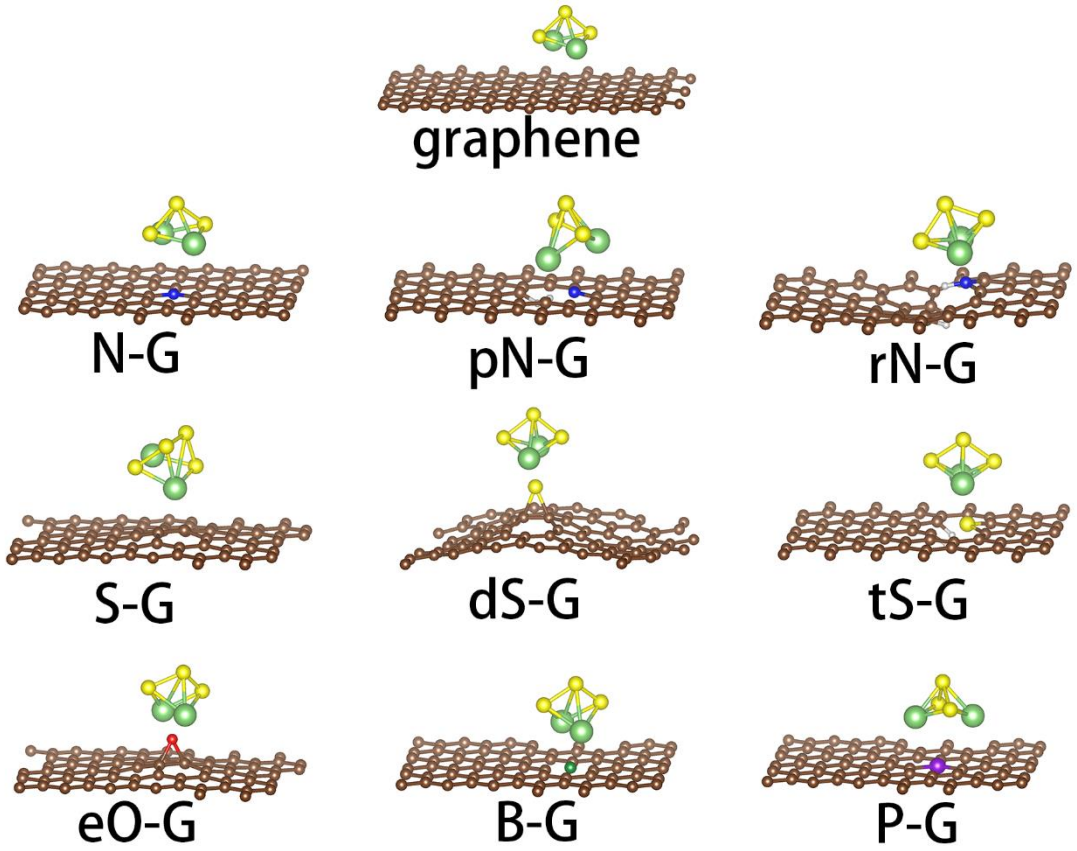

Fig. S3. Optimized F_1 adsorption configuration of graphene, N-G, pN-G, rN-G, S-G, dS-G, tS-G, eO-G, B-G, and P-G.

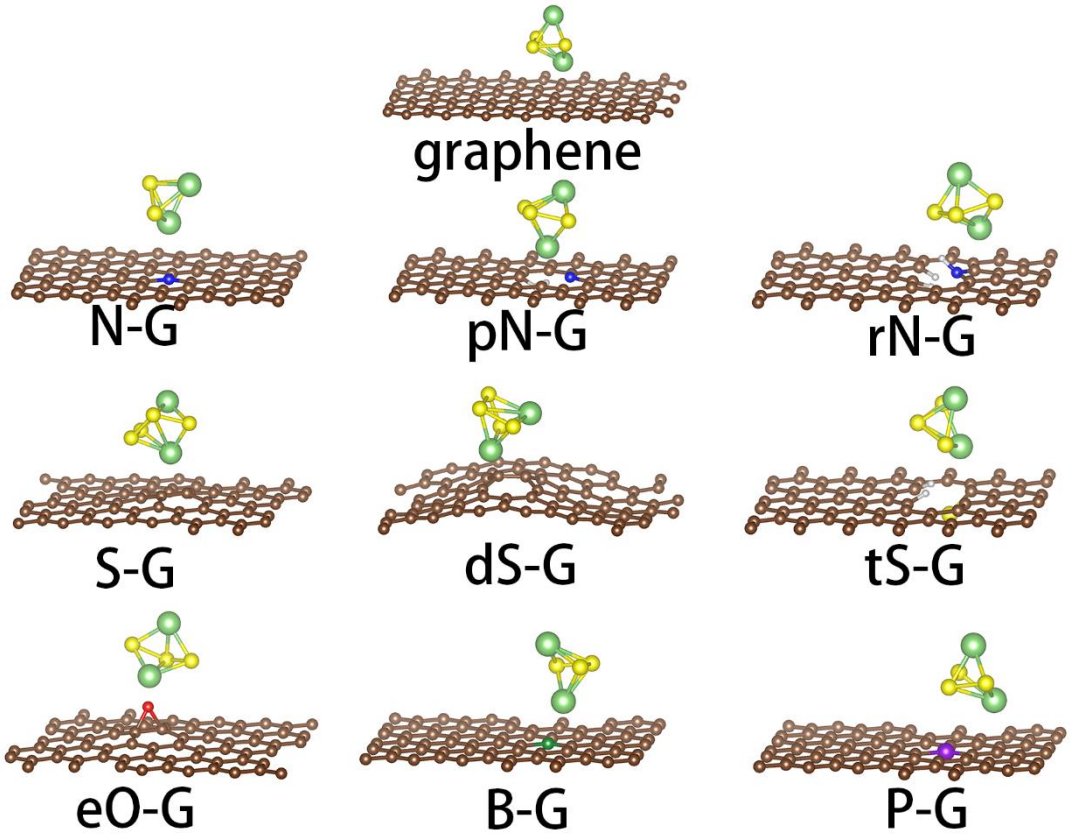

Fig. S4. Optimized F_2 adsorption configuration of graphene, N-G, pN-G, rN-G, S-G, dS-G, tS-G, eO-G, B-G, and P-G.

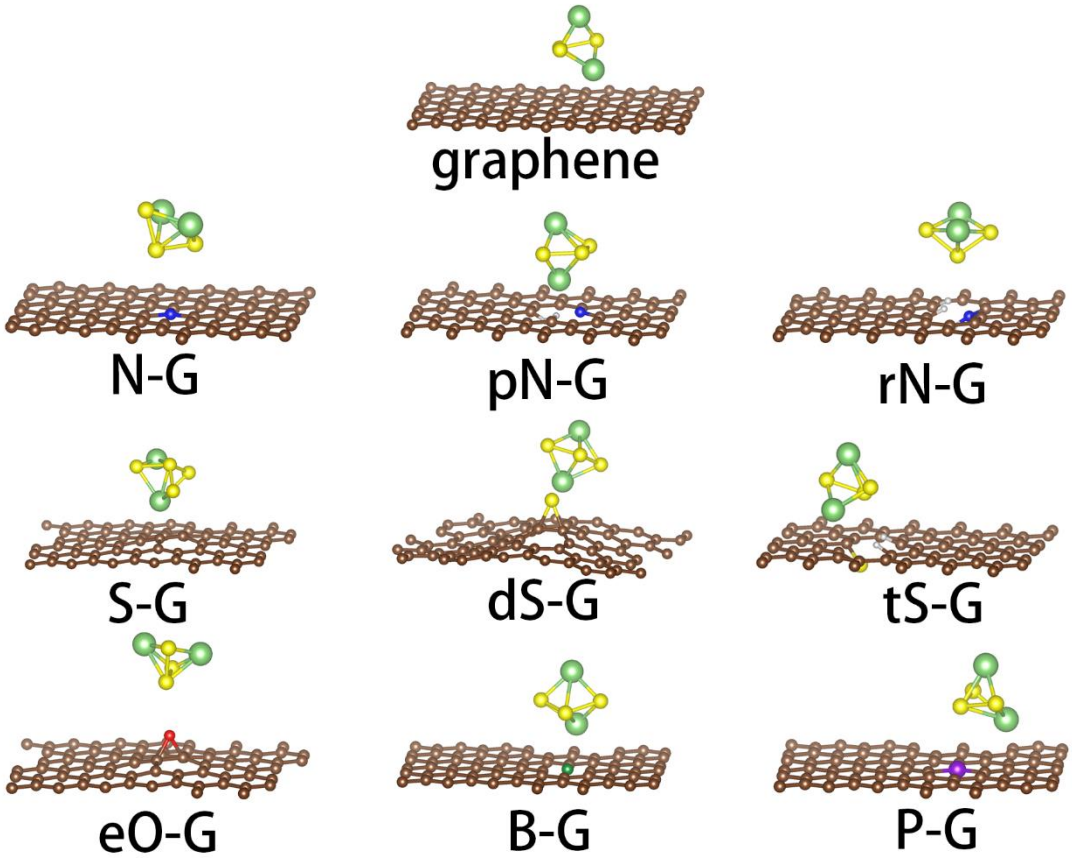

Fig. S5. Optimized F_3 adsorption configuration of graphene, N-G, pN-G, rN-G, S-G, dS-G, tS-G, eO-G, B-G, and P-G.

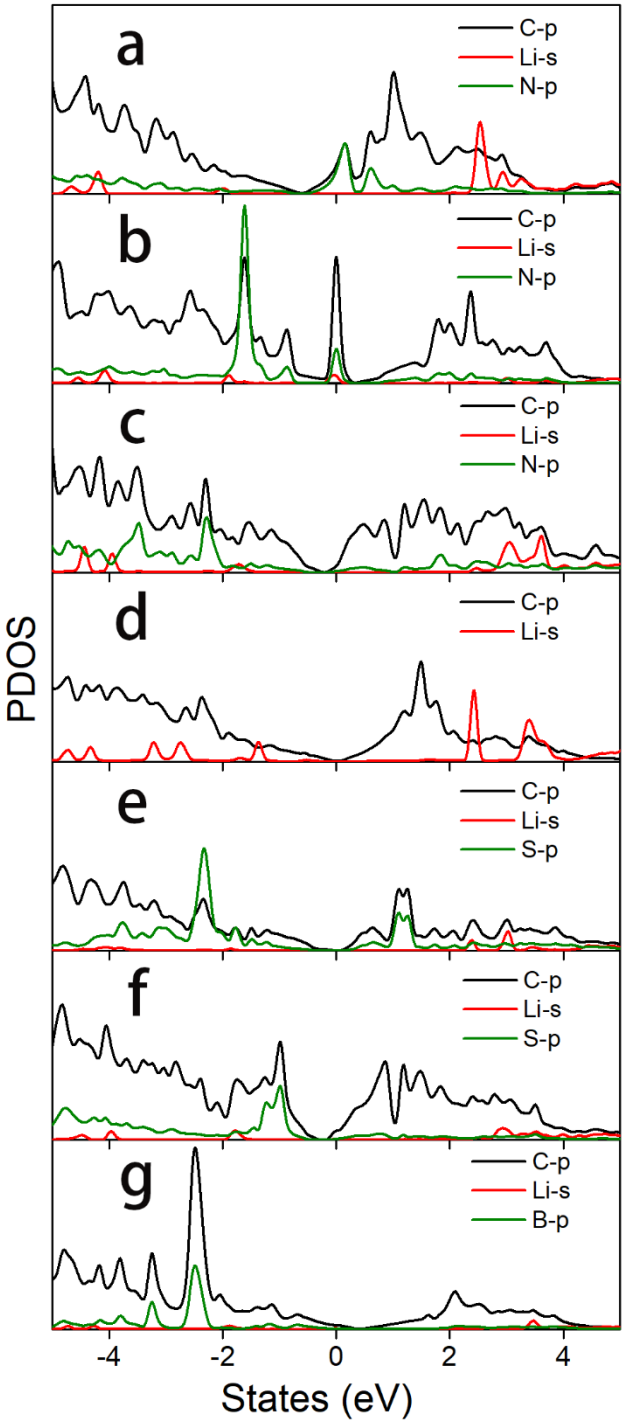

Fig. S6. Atomic projected density of state near Fermi energy region for Li_2S_3 adsorbing on the surface of (a) N-G, (b) pN-G, (c) rN-G, (d) S-G, (e) dS-G, (f) tS-G, (g) B-G.

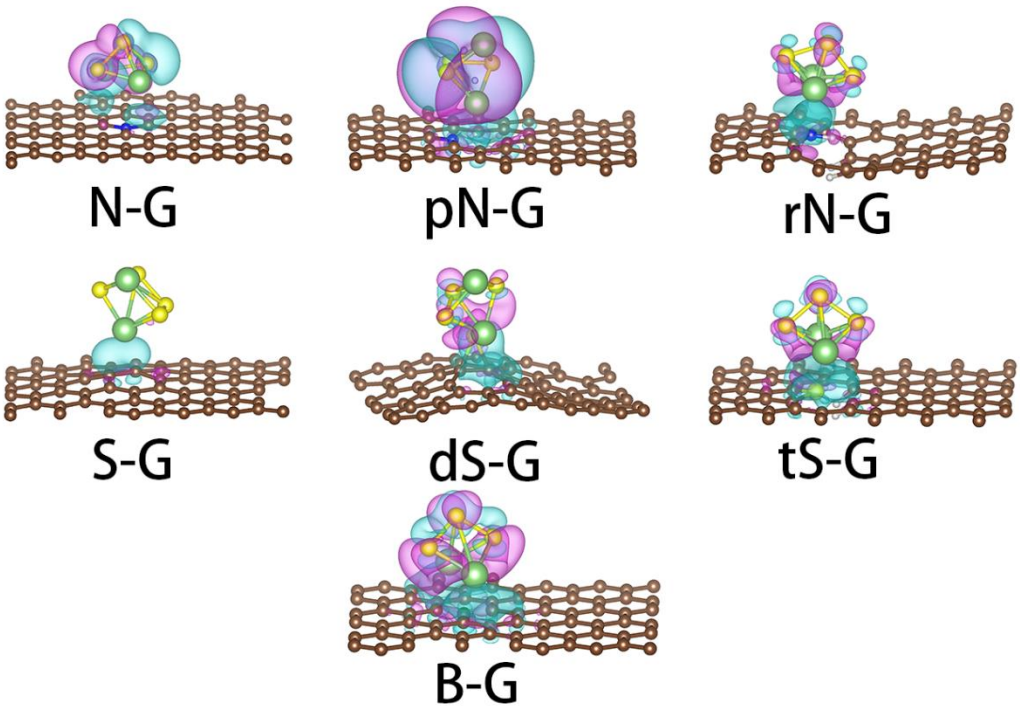

Fig. S7. The illustrations of charge density difference of Li_2S_3 adsorbing on the surface of (a) N-G, (b) pN-G, (c) rN-G, (d) S-G, (e) dS-G, (f) tS-G, (g) B-G, isosurface level is 0.0009 e $Å^{-3}$