The Anchoring Effect of 2D Graphdiynes Materials for Lithium-sulfur Batteries

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Supporting Information Available

- Table S1. Binding Energy (eV) of lithium PSs Li_2S_n ($n = 8, 6, 4, 2, 1$) clusters on GDYs materials calculated by GGA-PBE functional.
- Table S2. Binding energy (eV) of lithium PSs intermediates Li_2S_n ($n = 8, 6, 4$) on the bilayer (2L-) GDYs materials with vdW interaction.
- Figure S1. Potential of 1L- and 2L-γ-GY systems versus Z direction.
- Figure S2. The 3-dimensional charge density difference of Li_2S_n/GDY ($n = 8, 6, 4, 2, 1$) systems.

Table S1: Binding Energy (eV) of lithium PSs Li_2S_n ($n = 8, 6, 4, 2, 1$) clusters on GDYs materials calculated by GGA-PBE functional.

PSs	α-GY	β-GY	γ-GY	GDY	B-GDY
Li_2S_8	0.058	0.080	0.084	0.078	0.447
Li_2S_6	0.114	0.141	0.216	0.145	0.868
Li_2S_4	0.248	0.358	0.299	0.259	1.203
Li_2S_2	0.951	0.936	1.166	0.894	2.045
Li_2S	1.509	1.957	2.068	1.577	2.766

Table S2: Binding energy (eV) of lithium PSs intermediates Li_2S_n ($n = 8, 6, 4$) on the bilayer (2L-) GDYs materials with vdW interaction.

PSs	2L-α-GY	2L-β-GY	2L-γ-GY	2L-GDY
Li_2S_8	0.592	0.703	0.723	0.631
Li_2S_6	0.555	0.716	0.925	0.701
Li_2S_4	0.752	0.802	0.836	0.739

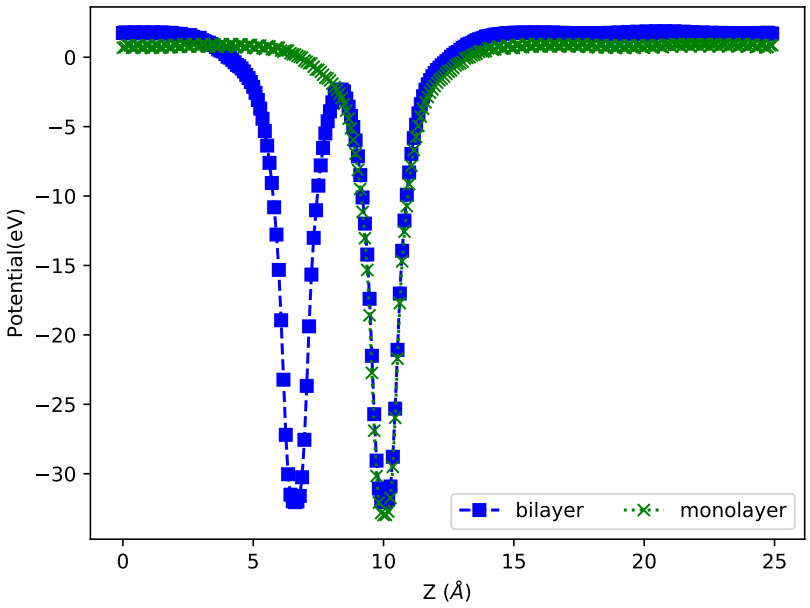
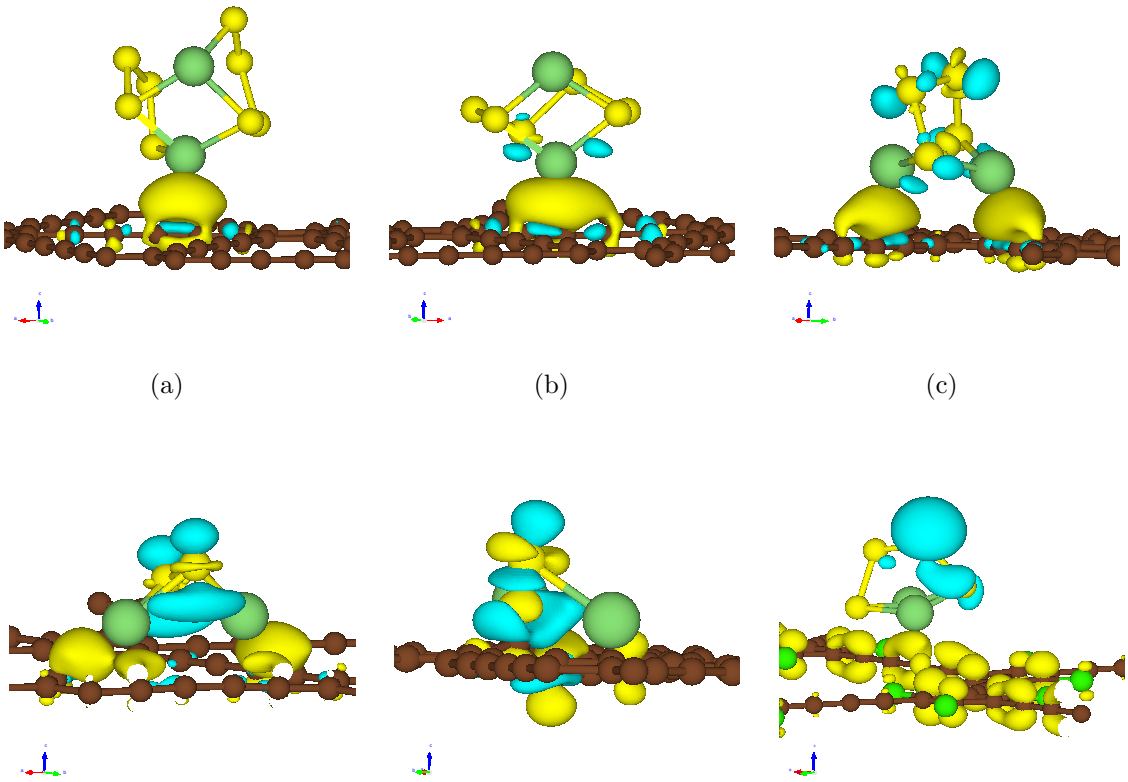


Figure S1: Potential of 1L- and 2L-γ-GY systems versus Z direction



(a) (b) (c)

(d) (e) (f)

Figure S2: The 3-dimensional charge density difference of Li_2S_n/GDY systems: (a)LiS_8/GDY, (b)LiS_6/GDY, (c)LiS_4/GDY, (d)LiS_2/GDY, (e)LiS/GDY, (f)Li_2S_4/Cl-GDY. In the Figure, the yellow and blue colors represent gaining and losing electrons respectively