Supporting Information

2D frameworks C_2N as potential cathode for lithium sulfur batteries: an ab initio density functional

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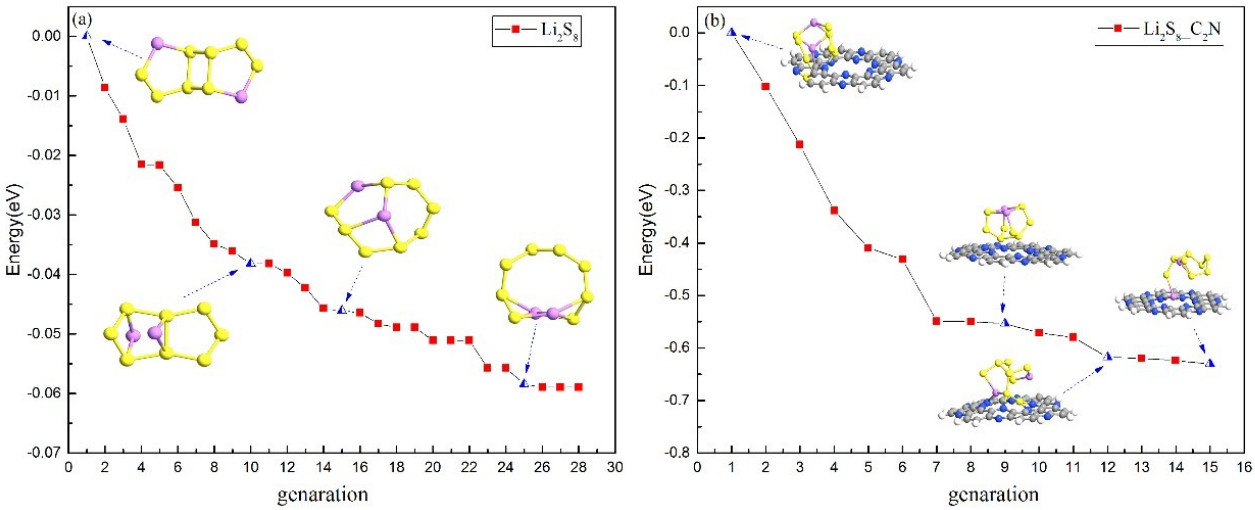

Fig.S1 Evolution of the best individual of population of one search of Li_2S_8 (a) and $Li_2S_8\_C_2N$ (b).

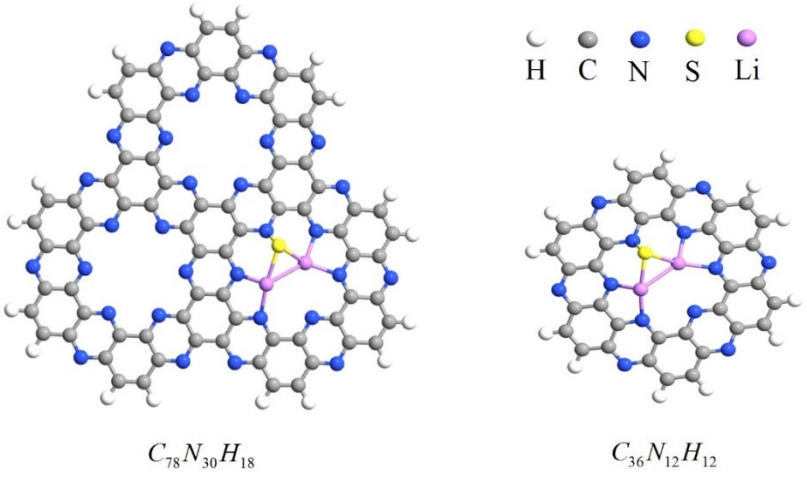

Fig. S2 Structure configures of $C_{78}N_{30}H_{18}$ (with three holes) and $C_{36}N_{12}H_{12}$ (with one hole) clusters

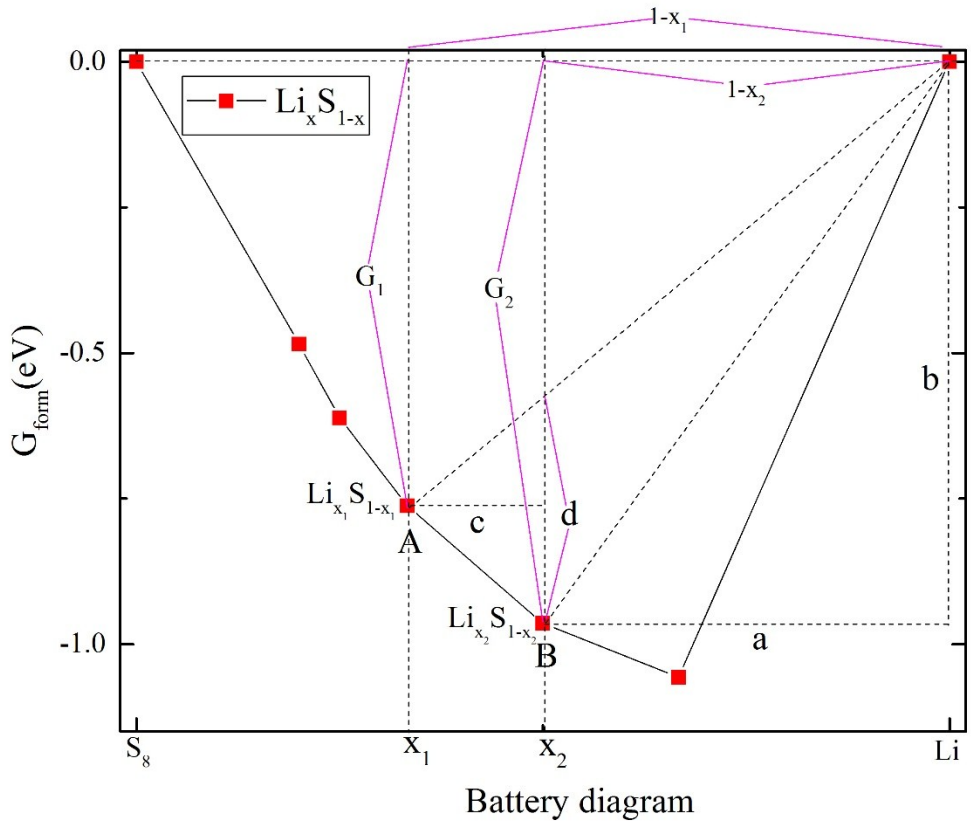

Fig. S3 the way to read the diagram of G_{form} :

(1) The reaction voltage

At the point A and B, there are two equations:

$$-G_1 = G(Li_{x_1}S_{1-x_1}) - (1-x_1)G(S_8)/8 - x_1G(Li)$$

$$-G_2 = G(Li_{x_2}S_{1-x_2}) - (1-x_2)G(S_8)/8 - x_2G(Li)$$

The voltage at x_1 :

$$V_1 = G_1 / x_1$$

The average voltage at x_2 :

$$V_2^a = G_2 / x_2$$

The lithiation From A to B:

$$\frac{1-x_2}{1-x_1}G(Li_{x_1}S_{1-x_1}) + \frac{x_2-x_1}{1-x_1}G(Li) = G(Li_{x_2}S_{1-x_2})$$

Where:

$$\frac{1-x_2}{1-x_1}\cdot x_1 \cdot V_1 + \frac{x_2-x_1}{1-x_1}\cdot V_2 = x_2 \cdot V_2^a$$

The voltage at x_2 :

$$V_2 = d \cdot \frac{1-x_1}{x_2-x_1} = d \cdot \frac{a+c}{c}$$

(2) The capacitance

The capacitance per S atom at x_1 :

$$C_1 = G_1 / (1 - x_1)$$

The additional capacitance per S atom from x_1 to x_2 :

$$\Delta C_{12} = d / (1 - x_2)$$

The total capacitance per S atom at x_2 :

$$C_2 = G_1 + \Delta C_{12}$$