

Supplementary Information

2D MoSi_2N_4 as electrode material of Li-air battery — A DFT study

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1. Some MoSi_2N_4 -Li structures

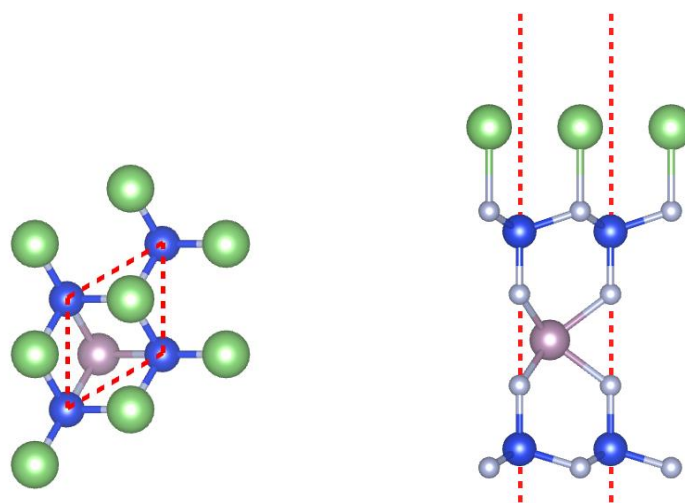


Fig. S1 The structure of MoSi_2N_4 with 100% Li coverage ($\text{Li}:\text{MoSi}_2\text{N}_4 = 1:1$, corresponding to **E** in **Fig. 2(a)**). Top and side views are shown.

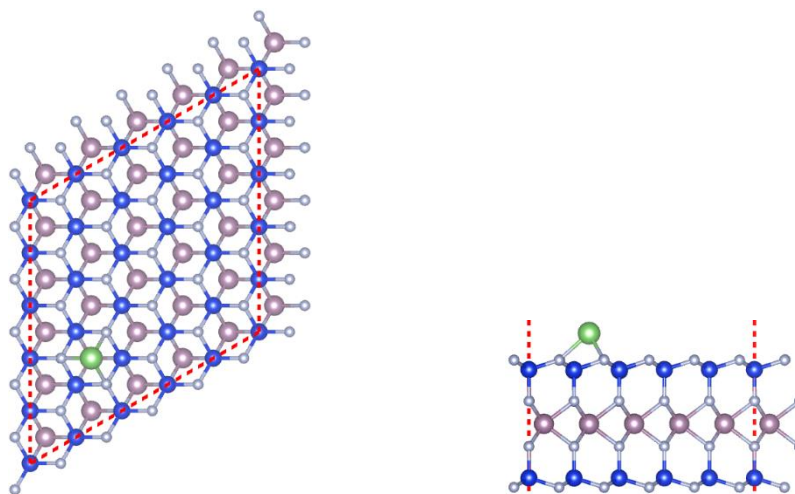


Fig. S2 The structure of MoSi_2N_4 with 4% Li coverage ($\text{Li}:\text{MoSi}_2\text{N}_4 = 1:25$, corresponding to **A** in **Fig. 2(a)**). Top and side views are shown.

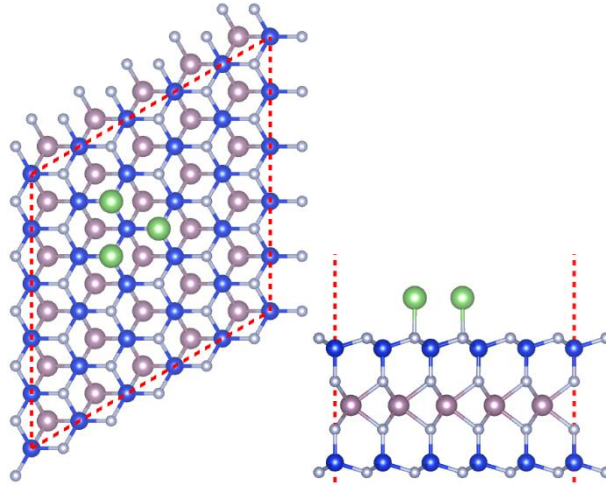


Fig. S3 The structure of MoSi_2N_4 with 12% Li coverage ($\text{Li}:\text{MoSi}_2\text{N}_4 = 3:25$, corresponding to **B** in **Fig. 2(a)**). Top and side views are shown.

2. Reaction coordinate

Fukui assumed that the atoms move along the minimal-energy path. For the mass-weighted coordinates $\xi_i = \sqrt{m_i}x_i$, we define

$$\frac{\Delta \xi_1}{\left(\frac{\partial E}{\partial \xi_1}\right)} = \frac{\Delta \xi_2}{\left(\frac{\partial E}{\partial \xi_2}\right)} = \dots = \frac{\Delta \xi_{3N}}{\left(\frac{\partial E}{\partial \xi_{3N}}\right)}$$

The reaction coordinate is the trajectory determined by the above equation.