Supporting Information

Nucleation and Conversion Transformations of the Transition Metal Polysulfide VS_4 in Lithium Ion Batteries

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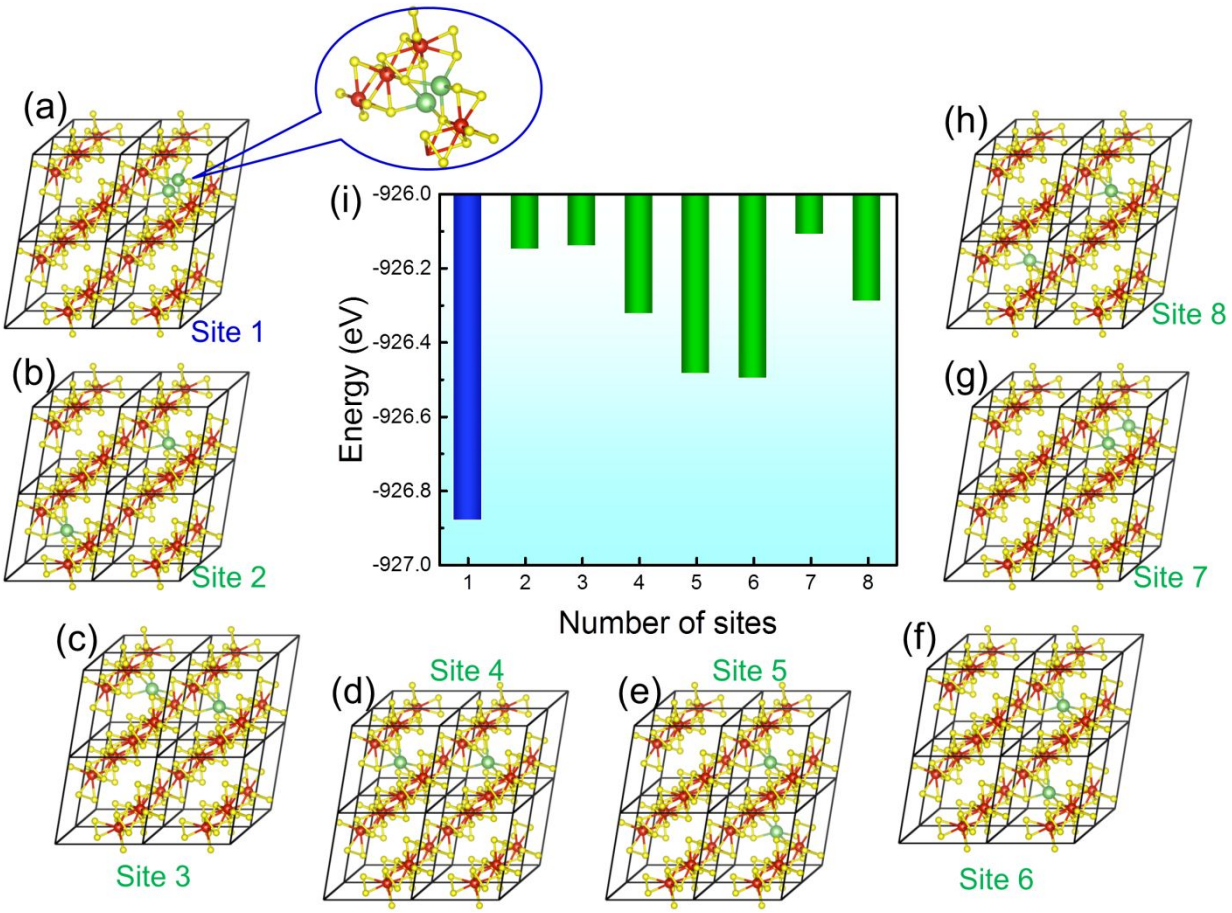

Fig. S1. The structures of a 2×2×2 VS_4 supercell with two Li atoms inserted in (a) a single unit cell; (b-h) different unit cells. (i) The total energy of these configurations. It showed that the aggregation model (Site 1) was indeed energetically favored.

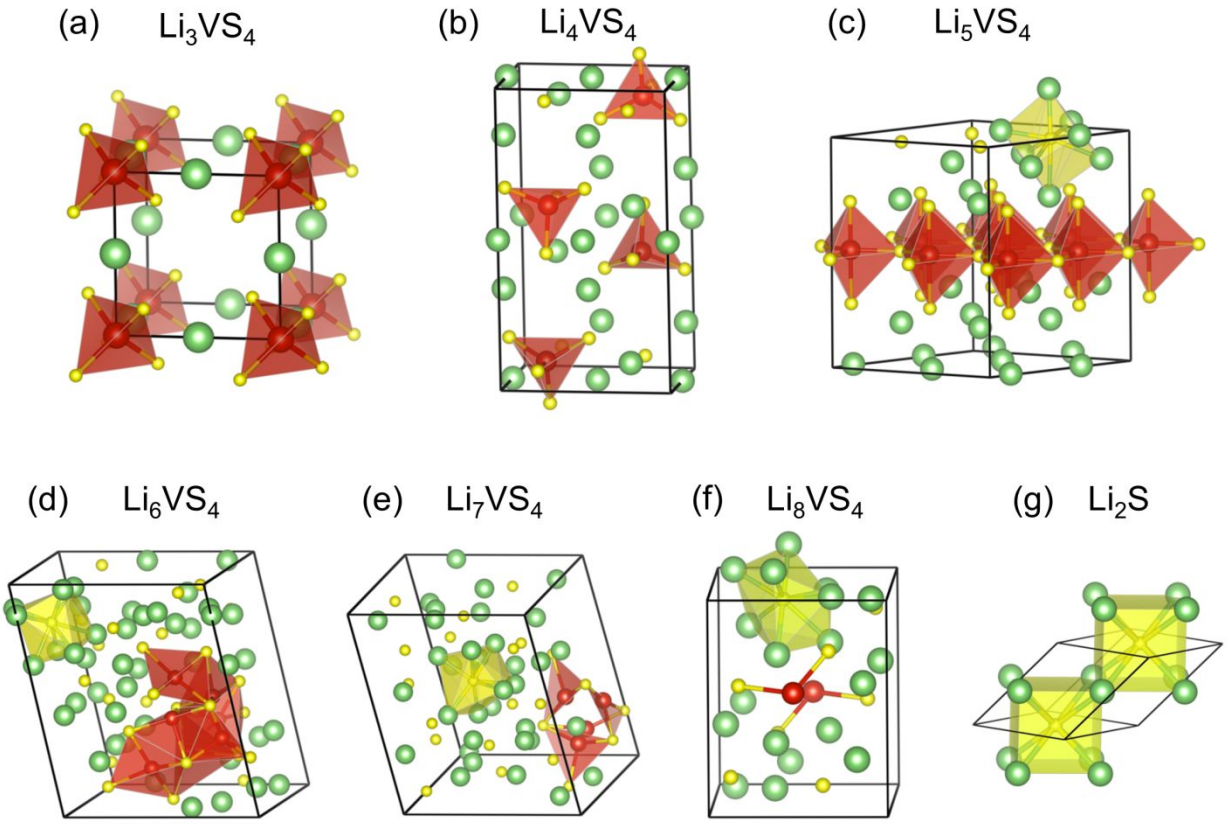

Fig. S2. (a-f) The predicted structures of Li_xVS_4 ($3 \leq x \leq 8$). (g) The crystal structure of Li_2S. It can be seen that the Li_8S cluster (yellow) formed in Li_xVS_4 ($5 \leq x \leq 8$) was different from the Li_8S unit in Li_2S crystal.

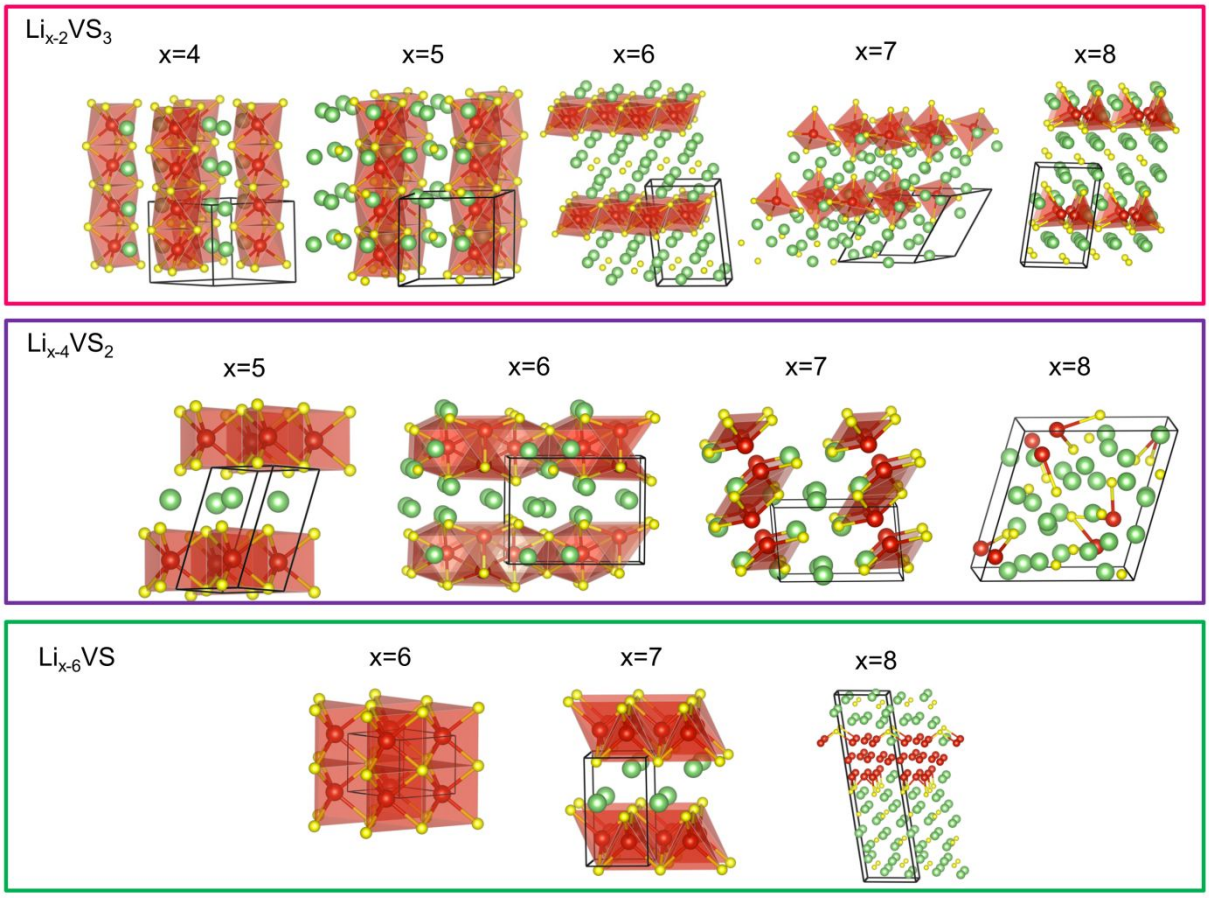

Fig. S3. The predicted structures of $Li_{x-2}VS_3$, $Li_{x-4}VS_2$ and $Li_{x-6}VS$ ($3 \leq x \leq 8$).

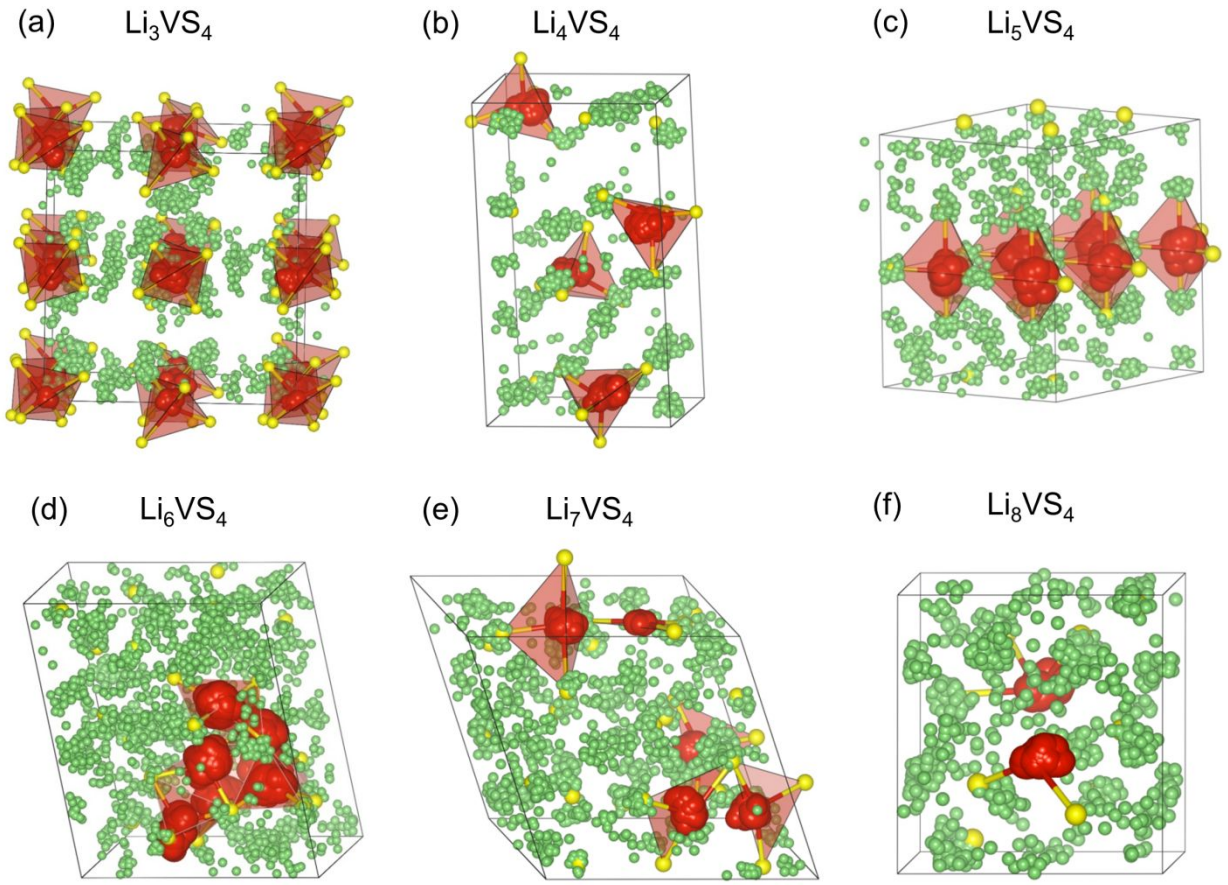

Fig. S4. The trace of Li^+ diffusion in the (a) Li_3VS_4, (b) Li_4VS_4, (c) Li_5VS_4, (d) Li_6VS_4, (e) Li_7VS_4, (f) Li_8VS_4 structure at 800K.