Supporting Information

Theoretical Study of Highly Efficient VS$_2$-based Single-Atom Catalysts in Lithium-Sulfur Batteries

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Fig. S1. Stable configurations of (a) Fe (b) Co (c) Ni (d) Ti (e) Sc on VS$_2$ monolayer.

Fig. S2. TDOSs and PDOSs of Fe@VS$_2$, Co@VS$_2$ and Sc@VS$_2$ monolayers. The Fermi level was set to zero.
**g. S3.** The most stable adsorption configurations of $L_2S_n$ and $S_8$ on (a) Fe@VS$_2$, (b) Co@VS$_2$, and (c) Sc@VS$_2$.
Fig. S4. Charge density difference of Li$_2$S$_n$ ($n = 1, 4, 8$) and S$_8$ on (a) Fe@VS$_2$ (b) Co@VS$_2$ (c) Ni@VS$_2$ and (d) Sc@VS$_2$.

Fig. S5. 2D slice of ELF for (a) Li$_2$S$_6$ and (b) Li$_2$S$_8$ adsorbed on Ti@VS$_2$ substrate. 2D slice of ELF for (c) Li$_2$S$_6$ and (d) Li$_2$S$_8$ adsorbed on Fe@VS$_2$ substrate.
Fig. S6. (a) The detailed decomposition path of Li$_2$S on Ni@VS$_2$. The diffusion pathways of lithium atom on (b) Ni@VS$_2$ (c) Sc@VS$_2$.

Fig. S7. PDOSs of VS$_2$ monolayer. Here, the PDOS by DS-PAW method (a) is consistent with that by Perdew–Burke–Ernzerh of exchange correlation function within the generalized gradient approximation (b).