Supporting Information

**Theoretical Study of Highly Efficient VS$_2$-based Single-Atom Catalysts in**

Lithium-Sulfur Batteries

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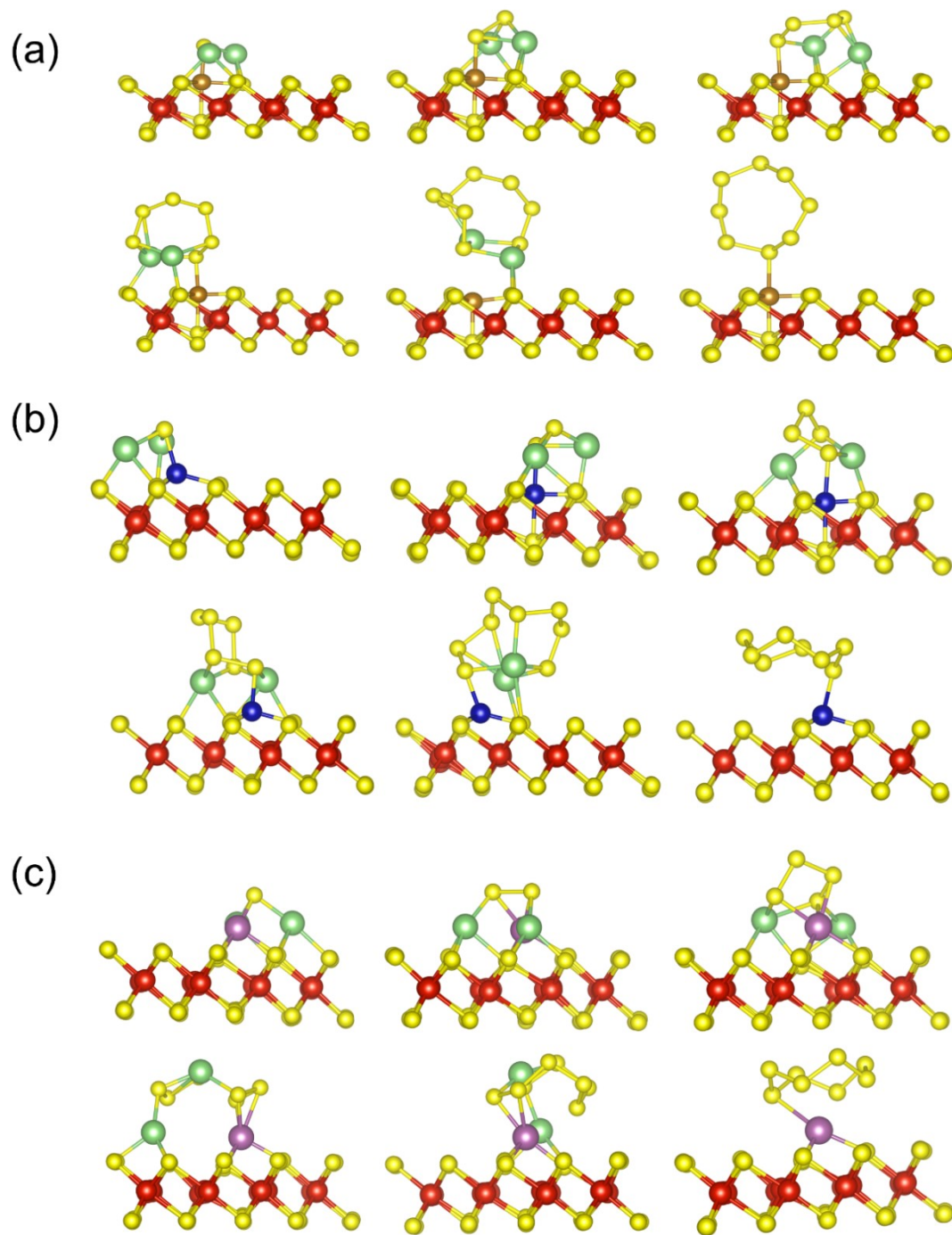
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Chemical and Biological Engineering, Zhejiang University, Hangzhou, 310027, China
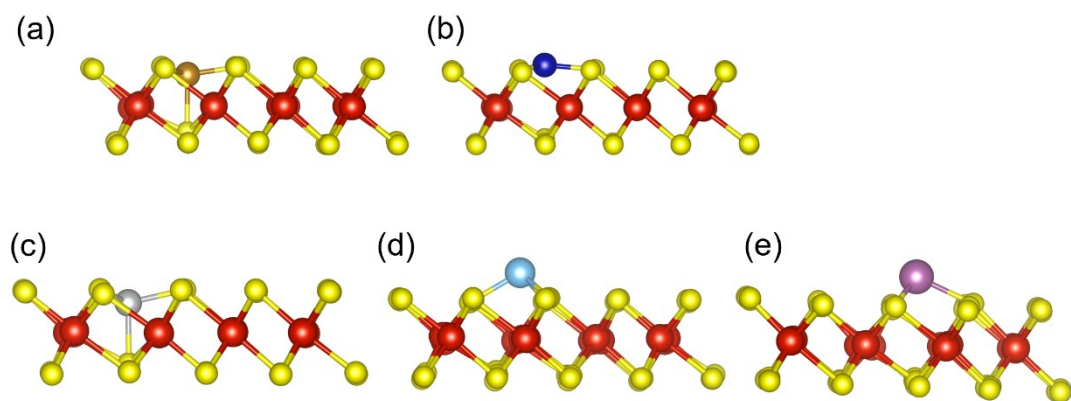
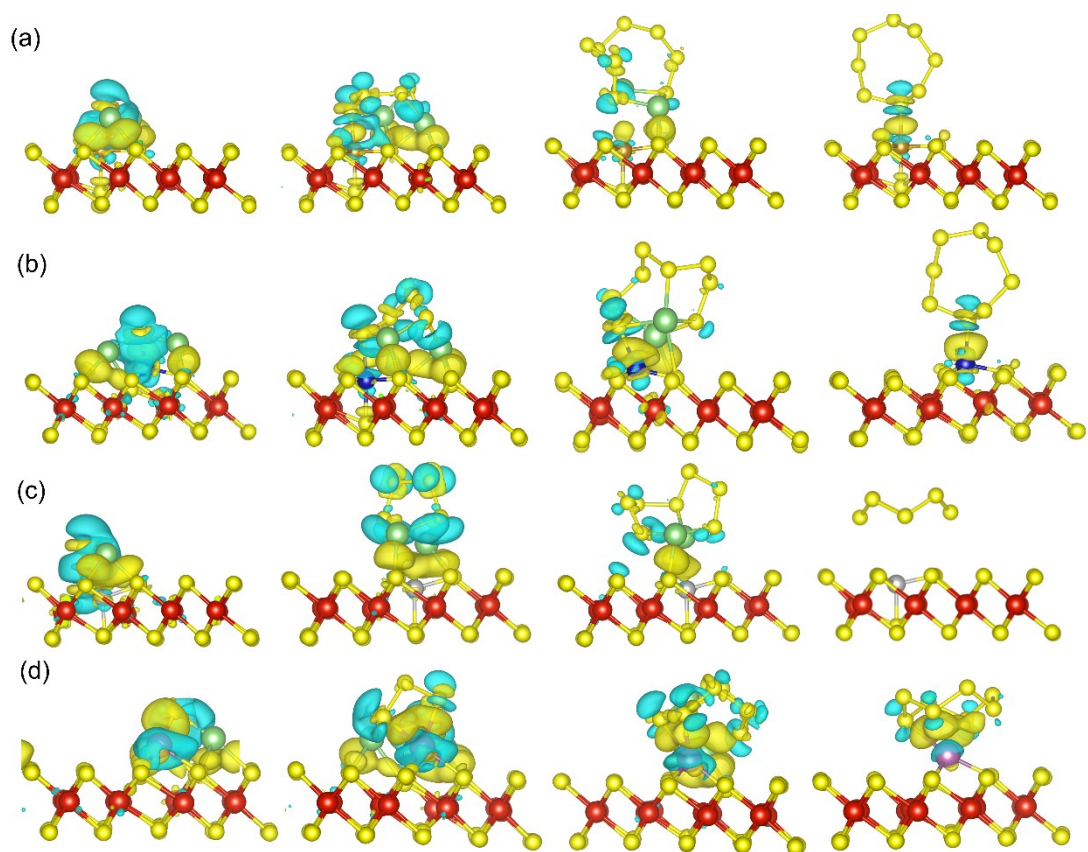**Fig. S1.** Stable configurations of (a) Fe (b) Co (c) Ni (d) Ti (e) Sc on VS$_2$ monolayer.
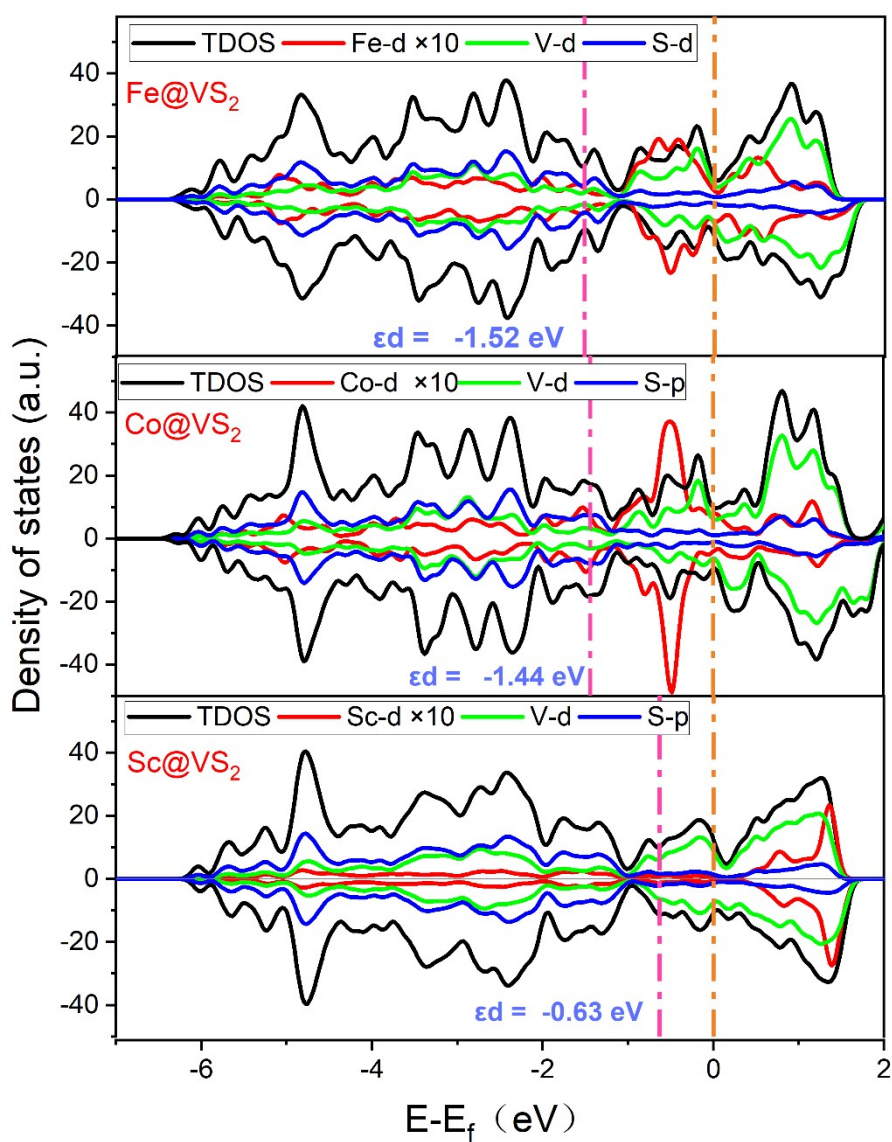
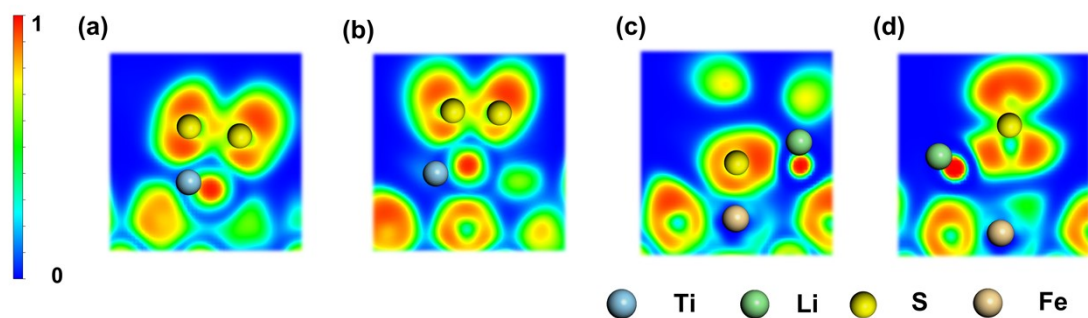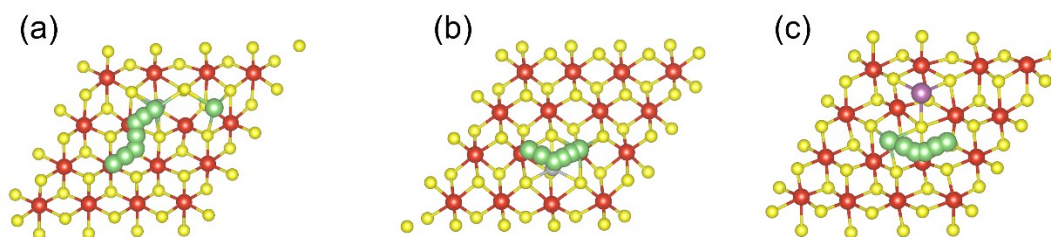**Fig. S2.** TDOSs and PDOSs of Fe@VS$_2$, Co@VS$_2$ and Sc@VS$_2$.

Fig. 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$_2$.
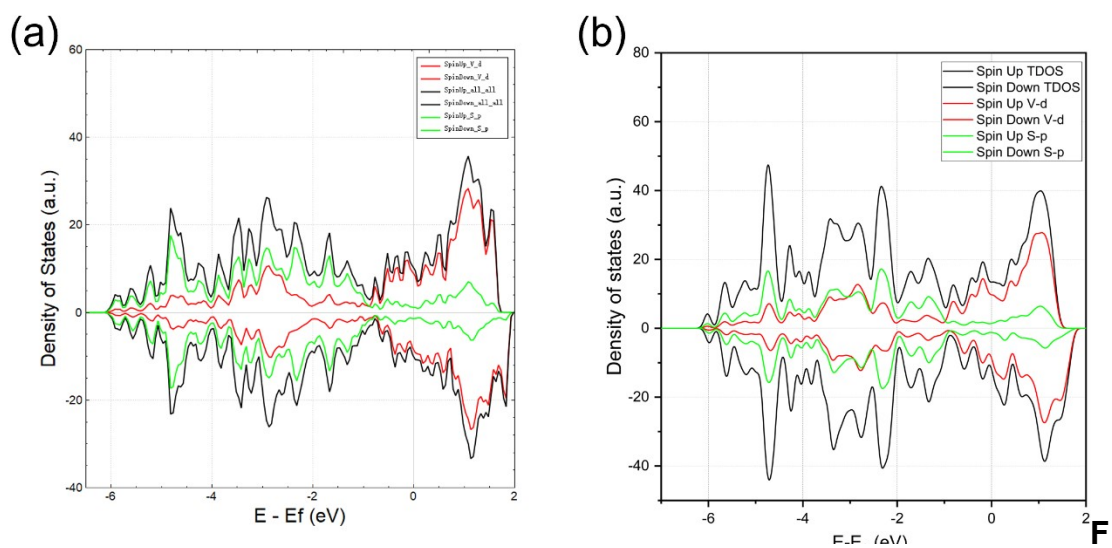
Fig. S4. Charge density difference of Li_2S_n (n = 1, 4, 8) and S_8 on (a) $Fe@VS_2$ (b) $Co@VS_2$ (c) $Ni@VS_2$ and (d) $Sc@VS_2$.

Fig. S5. 2D slice of ELF for (a) Li_2S_6 and (b) Li_2S_8 adsorbed on $Ti@VS_2$ substrate. 2D slice of ELF for (c) Li_2S_6 and (d) Li_2S_8 adsorbed on $Fe@VS_2$ substrate.

Fig. S6. (a)The detailed decomposition path of Li_2S on Ni@VS_2. The diffusion pathways of lithium atom on (b) Ni@VS_2 (c) Sc@VS_2.

ig. 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).