Anchoring and Electrocatalysis Effects of S-deficient $MoS_{2-\delta}$ for Li-S Batteries: Experiments and First-principles Calculations

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Lithium-sulfur (Li-S) batteries have been intensively investigated as one of the most promising next generation rechargeable batteries because of their high energy density. However, some serious shortcomings have impeded the practical applications of Li-S batteries, such as dissolution and shuttle effect of long-chained lithium polysulfide (Li_2S_n, n≥4) and low electronic conductivity of S and the short-chained Li_2S_2 and Li_2S species. In this work, using first-principles approach with van der Waals interaction, we demonstrated that S-deficient $MoS_{2-\delta}$ (2H) induced strong binding interaction with the Li_2S_n species. This strong chemical interaction effectively suppressed the shuttle effect of lithium polysulfides, resulting in larger discharge capacity, better cycle stability and rate capability. In addition, the S-deficient $MoS_{2-\delta}$ acted as an efficient catalyst for the Li_2S_n species by lowering the decomposition barriers of Li_2S_n particularly for Li_2S and Li_2S_2 which further improved the electrochemical performance of Li-S battery. The theoretical simulation results were well demonstrated by electrochemical experiments. This work presents a general guiding for the rational design of high performance Li-S batteries using transitional metal disulfides as electrode additives.

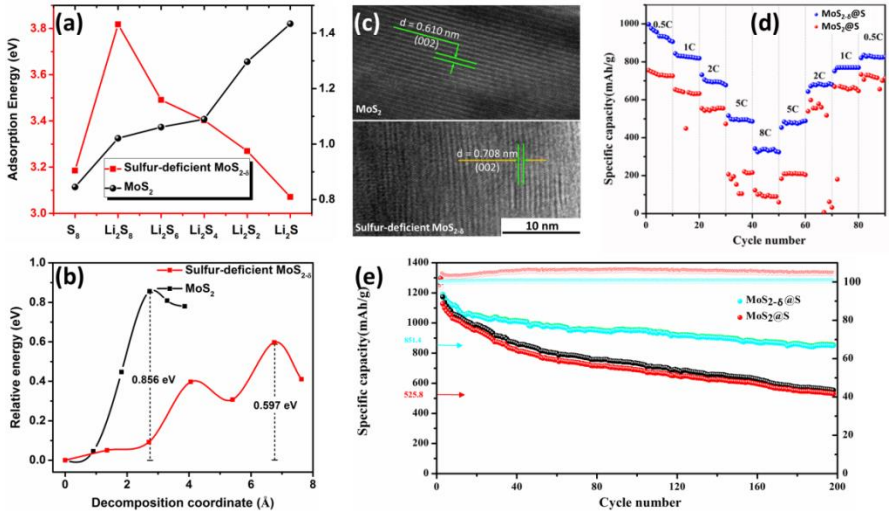

Fig 1. (a) Binding energies of Li_xS_n at different lithation stages on sulfur-deficient $MoS_{2-\delta}$ and intact MoS_2; (b) Energy profiles for decomposition of Li_2S on $MoS_{2-\delta}$ and MoS_2. (c) HRTEM images of $MoS_{2-\delta}$ and MoS_2; (d) Rate performance and (e) cycling performance of $MoS_{2-\delta}$ and MoS_2.

References:

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