Theoretical Insights into the Conversion Mechanism of Li2S2 to Li2S in Lithium-Sulfur Batteries based on VO(1-x)S(1+x) Alloys

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Abstract

Lithium-sulfur batteries are regarded as the most promising energy storage system due to their high theoretical capacity (1675 mAh/g) and natural abundance of elemental sulfur. Nevertheless, the sluggish reaction of the rate-limiting step Li $_2$S $_2$ to Li $_2$S conversion severely hampers the practical application of lithium-sulfur batteries. The resolution of this issue is contingent upon a thorough comprehension of the conversion mechanism of the rate-limiting step. To this end, we have developed the two-dimensional VO $_{(1-x)}$S $_{(1+x)}$ alloy catalysts by ATAT and have constructed a theoretical model that can accurately predict the thermodynamic energy barrier of the rate-limiting step in lithium-sulfur batteries. Our model relates the energy barrier of the rate-limiting step to the *p*-band center of the nonmetallic and the *d*-band center of the metallic for the VO $_{(1-x)}$S $_{(1+x)}$ alloy. This model facilitates the identification of the VO $_{(1-x)}$S $_{(1+x)}$ alloy as a potential cathode catalyst for lithium-sulfur batteries.

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