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ACCEPTED MANUSCRIPT

Promoting Lithium Polysulfide/sulfide Redox Kinetics by the Catalyzing of Zinc

Sulfide for High Performance Lithium-Sulfur Battery

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Abstract: Entrapping polysulfide from dissolution into electrolyte by strong chemisorption of polar materials has been widely reported in lithium-sulfur (Li-S) battery. Here, for the first time, zinc sulfide (ZnS) was demonstrated as an activation catalyst in Li-S battery to suppress the soluble polysulfide shuttle effect by powering redox reactions kinetics lithium polysulfide/sulfide. Kinetic of analyses comprehensively identify that ZnS not only facilities polysulfide redox kinetics in liquid phase (Li₂S₈ \rightarrow Li₂S₆ \rightarrow Li₂S₄), but also promotes the effective decompositions of lithium sulfide (Li₂S). Furthermore, first-principle calculations confirm that the low lithium ion diffusion barrier on the surface of ZnS promotes the redox reaction between lithium ion and sulfur species; and the low migration energy barrier of polysulfide on its surface guarantees the fast diffussion of polysulfides from the ZnS

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