Density Functional Theory Studies on Tuning TaXTi(1-X)S2 For Insoluble Li2S2-Li2S Conversion in Lithium-Sulfur Batteries

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Abstract

Due to the complexity of insoluble Li2S2-Li2S conversion, few descriptors exist to correlate the catalytic performance and the underlying electronic structures of a given catalyst, which inhibits the development of lithium-sulfur catalysts. In this article, we employ the cluster expansion method to select 17 optimal structures for TaXTi(1-X)S2 (0[?]X[?]1) and apply density functional theory calculations to probe the electronic structures and the conversion of Li2S2 to Li2S relationships across different doping concentrations. We found the simultaneous pathway is most possible in propose five possible reaction pathways. Notably, we identify Ta0.38Ti0.62S2 as a promising candidate for electrocatalytic applications in the conversion from Li2S2 to Li2S. Furthermore, our study analyzes the charge transfer of Li2S2(QLi2S2)), the electronegative difference(ΔX), the adsorption energy of Li2S(EaLi2S)), and work function(WF) significantly influence the conversion process from Li2S2 to Li2S by machine learning based on various descriptors. This research contributes to a deeper theoretical understanding of the complex mechanisms underlying the Li2S2-Li2S conversion and provides valuable insights into the rational design of sulfur redox catalysts.

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