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Co₃O₄ SURFACE STUDIES AND ADSORPTION OF Li₂O₂ NANOCUSTER

ABSTRACT

Lithium-air batteries represent one of the most promising technologies for energy storage, characterized by their high energy density (1086 Wh/kg) and substantial specific capacity (3842 mAh/g). However, they experience a practical drawback that involves the production of unstable discharge products (LiO₂, Li₂O and LiO) resulting in battery degradation. Cobalt oxide (Co₃O₄) is considered an effective electrocatalyst for Li-air batteries because of its mixed Co²⁺ and Co³⁺ oxidation states which reduce over-potential and significantly improve the cyclic performance of a Li-O₂ battery. Despite that, there is a limited understanding of the adsorption of stable discharge products (Li₂O₂) on major Co₃O₄ surfaces. In this work, we use the density functional theory (DFT) method to investigate the surface properties and the adsorptions of Li₂O₂ nanocluster to mimic the growth of the discharge product on the major surfaces. Thus, the (001) surface was found as the most stable among the three low Miller indexes (i.e., (001), (011) and (111)) surfaces. The constructed Wulff Morphology was compatible with the previous studies, with a dominance of the (001) plane. The discharge Li₂O₂ nanocluster were then adsorbed on the (001) surface and the results shows that the nanocluster favors to bridge across the Co²⁺ and Co³⁺ with the adsorption energy of E_{ads} = -4.147 eV. The findings for this research will help us better understand the production of Li₂O₂ and its interactions with the Co₃O₄ electrocatalyst.

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