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# Co3O4 SURFACE STUDIES AND ADSORPTION OF Li2O2 NANOCLUSTER

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 Eads = -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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