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Computational Study bulk and Surface RuO2 as a catalyst in Li-air Batteries

Lithium-air batteries have long been regarded as one of the best choices due to their high specific energy (11,400 Wh/kg). Catalysis is one of the most effective techniques used to improve electrochemical performance and influence the production of stable discharge products during cycling in lithium-air batteries. Despite several studies addressing the effect of catalysis in Li-air batteries, the reactivity and catalytic effect of ruthenium oxide (RuO2) are not fully understood. In acidic conditions, RuO2 performs exceptionally well and lasts a long time in the oxygen evolution reaction(OER). Ru-based catalysts are generally considered to be the most efficient oxygen reduction reaction (ORR) catalysts. In this study, we use first principle density functional theory calculations to investigate the surface study of RuO2. Which will form a foundation for adsorptions of lithium and coadsorptions of oxygen. The B/G ratio is greater than 1.75 implies RuO2 is ductile. All the elastic constants were determined to be positive, indicating that the RuO2 is mechanically stable. Low Miller index {(001), (100), (010), (011), (110), (111)} surfaces were modelled, and we found the (110) surface to be the most stable. The constracted morphologies also indicated the (110) surface plane as the most dominant.

Keywords: Lithium-air batteries, Catalyst, oxygen evolution reaction(OER), oxygen evolution reaction(OER), Density functional theory(DFT),

Apply to be considered for a student ; award (Yes / No)?

Yes

Level for award;(Hons, MSc, PhD, N/A)?

Hons

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