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Exploring the effectiveness of RuO2 os a catalyst in metal-air batteries

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 effectiveness of catalysts in Li-air batteries, the reactivity and catalytic effect of ruthenium oxide (RuO2) are not fully understood. In this study, we used the first principle density functional theory calculations to inverstigate the adsorption of lithium and oxygen adsorptions towards the RuO2 major surface. 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. Considering the unique redox property of RuO2, the will turn to influence the production of stable discharge products upon cycling.

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