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Ab-Initio Study of Stability of Discharge Products in Li/Na-Air Batteries

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Rechargeable metal-air batteries have attracted a growing interest due to their significantly higher theoretical energy density. It is well recognize that the performance of the battery is governed by the electrochemical reactions that occur at the cathode which result in the formation of discharge products. Different discharge products are produced, through the Oxidation Reduction Reaction (ORR), and among those products some are unstable which might react with other components of the battery contribute to the capacity fading and aging. First principle density functional theory (DFT) was used to investigate the stability of discharge products. We found that LiO₂ marcasite is stable and NaO₂ is slightly stable due to the absence of soft mode along the Γ-direction in the phonon dispersion curve. Ceder et al. previously investigated the nanoscale stabilization of sodium oxides and found NaO₂ to be metastable at standard conditions and also found that LiO₂ marcasite is stable. Our results are aimed to give an insight on the stability of major discharge products and give research direction towards controlling the formation of desired Li/Na-O compounds in the batteries.

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