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POTENTIAL MANGANESE OXIDE (MNXOY) CATALYSTS FOR OXYGEN REDUCTION REACTION (ORR)

Today, lithium ion batteries (LIBs) dominate the rechargeable battery market despite their limitations, including low energy storage density (100–200 Wh/kg), high cost, potential supply shortages, and safety risks due to the flammability of lithium and organic electrolytes. Metal-air batteries (MABs) offer a high energy density, ranging from 400 to 1700 Wh/kg. However, the Fe-air battery (764 Wh/kg) received more attention due to its cost-effectiveness, eco-friendly nature, and for being less susceptible to dendrite formation, enhancing their safety and longevity. Despite that, Fe-air batteries encounter challenges related to their low-rate capability, cycling life and side chemical reactions resulting in battery deterioration. In this work, density functional theory (DFT) study is employed to investigate the structural, mechanical and electronic properties of potential MnxOy bulk catalysts. The calculated lattice parameters and elastic constants compared well with those obtained experimentally, with the percentage difference of 2%. The total density of states (TDOS) indicate the MnO2 system as the most stable as compared to Mn2O3 and Mn3O4.These findings give insight in improving the life cycle and over-potential of the battery.

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