Abstract Submitted
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First-Principles Study of Hydrogen Trapping in Electrolytic Manganese Dioxide[1] BIRENDRA ALE MAGAR, New Mexico State University, TIMOTHY N. LAMBERT, JONATHON DUAY, BABU CHALAMALA, Sandia National Laboratories, IGOR VASILIEV, New Mexico State University — Alkaline Zn/MnO_2 batteries hold great promise for electrical energy storage due to their high energy density, non-toxicity, and low cost. At a low depth of discharge, the reduction reaction in the Zn/MnO_2 battery cathode is governed by hydrogen trapping in the solid phase of γ-MnO_2. We applied ab initio computational methods based on density functional theory to study the mechanism of hydrogen insertion into the pyrolusite and ramsdellite tunnels of γ-MnO_2. Our calculations were carried out using the Quantum ESPRESSO electronic structure code combined with Vanderbilt ultrasoft pseudopotentials. We found that the trapped hydrogen initially occupied the 2×1 ramsdellite tunnels of γ-MnO_2. Our study showed that the insertion of hydrogen into the 1×1 pyrolusite tunnels induced significant structural distortions leading to the breakdown of the crystal structure of γ-MnO_2. These results could explain the presence of groutite and the absence of manganite among the reaction products of partially reduced γ-MnO_2.

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