First-Principles Study of the Surface Properties of ZnO Anode Material in Rechargeable Zn/MnO_2 Batteries*

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Zinc electrodes show promise for grid-scale energy storage systems because of their high theoretical capacity, stability, non-toxicity, and low cost. The performance of zinc anodes in aqueous alkaline batteries is affected by the structure and composition of a solid-state layer of ZnO grown on the surface of metal Zn. Recent studies have shown that the crystal structure of ZnO formed in zinc anodes could contain a large number of defects and impurities, such as O and Zn vacancies and interstitial hydrogen. The presence of defects and impurities in the structure of ZnO has a significant impact on the electrochemical properties and rechargeability of zinc anodes. We apply *ab initio* density functional computational methods to investigate the mechanisms of defect formation in the bulk and on the surface of ZnO. Our calculations show that the formation energies of O and Zn vacancies near the surface of ZnO are significantly lower than those in the bulk ZnO. The energies of hydrogen atoms attached to the surface of ZnO are found to be approximately 0.7 – 1.4 eV lower than the energies of hydrogen atoms inserted into the bulk ZnO. The results of our study suggest that the surface regions of ZnO have a strong influence on the electrochemical properties of zinc anodes.

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