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Ab Initio Study of the Influence of Structural Defects on the Electrochemical Properties of MnO_2 in Rechargeable Zn/MnO_2 Alkaline Batteries[1] NIRAJAN PAUDEL, BIRENDRA MAGAR, Department of Physics, New Mexico State University, Las Cruces, New Mexico 88003, USA, TIMOTHY LAMBERT, Department of Materials, Devices, and Energy Technologies, Sandia National Laboratories, Albuquerque, New Mexico 87185, USA, IGOR VASILIEV, Department of Physics, New Mexico State University, Las Cruces, New Mexico 88003, USA — The performance of MnO_2 electrodes in rechargeable solid-state alkaline Zn/MnO_2 batteries can be enhanced by nanostructuring and by introducing cation and oxygen vacancies into the crystal structure of MnO_2. However, the mechanism of this enhancement has not been investigated in detail. We apply *ab initio* density functional computational methods to study the mechanism of hydrogen ion insertion into the structures of β-, R-, and γ-MnO_2 polymorphs containing cation vacancies, oxygen vacancies, and surfaces. Our calculations show that the presence of bulk defects and surfaces significantly changes the binding energies of hydrogen ions inserted into the crystal structures of MnO_2 polymorphs. The results of our study show that surfaces and structural defects have a strong influence on the electrochemical properties of MnO_2.

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