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Bi- and Cu-Modified δ-MnO_2 Electrodes in Rechargeable Zn/MnO_2 Batteries: An *Ab Initio* study.[1] BIRENDRA ALE MAGAR, NIRAJAN PAUDEL, Department of Physics, New Mexico State University, Las Cruces, New Mexico 88003, TIMOTHY N. LAMBERT, Department of Materials, Devices, and Energy Technologies, Sandia National Laboratories, Albuquerque, New Mexico 87185, IGOR VASILIEV, Department of Physics, New Mexico State University, Las Cruces, New Mexico 88003 — Despite experimental evidence of the influence of Bi and Cu additives on the performance of rechargeable Zn/MnO_2 batteries, the mechanism by which these additives affect the rechargeability and cyclability of the δ-MnO_2 electrode has not been explained in detail. We apply first-principles computational methods based on density functional theory to study the electrochemical properties of Bi- and Cu-modified delta-MnO_2 electrodes in rechargeable Zn/MnO_2 batteries. Our calculations show the possibility of formation of Bi-Mn and Cu-Mn oxides in Bi/Cu-modified δ-MnO_2 cathodes during battery cycling. The results of our study suggest that the formation of intermediate Bi-Mn and Cu-Mn oxides could reduce the rate of accumulation of irreversible redox reaction products in the MnO_2 electrode.

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