Abstract: NeSA202100poster-06: MnO_2 Cathodes Modified with Bi, and Cu: A Great Promise for Electrical Energy Storage and Power Grid Applications.

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Presenter:

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Rechargeable alkaline Zn/MnO_2 batteries hold great promise for electrical energy storage and power grid applications due to their high energy density, non-toxicity, and low cost. Bi and Cu additives are known to significantly extend the cycle life and increase the capacity of MnO_2 electrodes in rechargeable Zn/MnO_2 batteries. However, the mechanism of interaction of Bi and Cu with the MnO_2 cathode material is not completely understood. To investigate the influence of chemical additives on the rechargeability and cyclability of MnO_2 electrodes, we calculated the geometries and formation enthalpies for a wide variety of crystal structures of MnO_2 modified with Bi, Cu, and Mg using *ab initio* computational methods based on density functional theory. The results of our calculations suggest that reversible transitions between the layered and spinel phases could play an important role in the cycling mechanism of chemically modified MnO_2 cathodes.