

Abstract Submitted
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Density Functional Theory Study of the Conductivity of Manganese Dioxide Nanowires during Li⁺ Insertion¹ RUQIAN WU, Department of Physics and Astronomy, University of California, Irvine, CA 92697, USA, HUI WANG, Department of Physics, Fudan University, Shanghai 200433, China, MAY LE THAI, REGINALD M. PENNER, Department of Chemistry, University of California, Irvine, CA 92697, USA — Manganese oxide (δ -MnO₂) as a battery material has various advantages such as low cost, high earth abundance and environmentally safe, and it has large interlayer space for lithium ion insertion and migration. In this work, the system of 200 MnO₂ nanowire array is used to study the electrochemical changes through in situ conductivity measurements during the lithium ion insertion process. The result indicates that the conductivity of each MnO₂ nanowire array increases as the lithium ion concentrations increases corresponding to more negative insertion potential. We perform *ab initio* molecular dynamic (AIMD) simulations and density functional theory (DFT) calculations with the van der Waals (vdW) correction to understand the fundamental electrochemical and structural properties of δ -MnO₂ nanowires. We find that water molecules are important for the expansion of the interlayer distance of δ -MnO₂, and reveal that the variation of conductivity of δ -MnO₂ nanowires with different Li⁺ concentrations stems from the Li-produced gap states.

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