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Uncovering the intrinsic delithiation mechanism in Li-excess Li_2MnO_3 through defect calculations KHANG HOANG, North Dakota State University — Layered Li-excess Li_2MnO_3 has been of great interest for lithium-ion battery cathodes because of its high theoretical capacity. The compound is also an important component in $x\text{Li}_2\text{MnO}_3 \cdot (1-x)\text{LiMO}_2$ and other high-capacity cathode materials. It has been reported that Li_2MnO_3 can be made electrochemically active by acid leaching or charging to high voltages. Several different mechanisms have been proposed to explain its unconventional lithium extraction behavior, including one that involves oxidation at the oxygen site. In this talk, we will present a comprehensive computational approach based on first-principles hybrid density functional defect calculations, and illustrate how it helps uncover the defect physics and chemistry and the intrinsic mechanisms for delithiation and electronic and ionic conduction in layered Li_2MnO_3 . In light of our results, we discuss the relevance of the proposed mechanisms and suggest solutions for improving the electronic conduction and hence the electrochemical performance of Li_2MnO_3 and related materials.

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