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Defect physics vis-à-vis electrochemical performance in layered mixed-metal oxide cathode materials KHANG HOANG, North Dakota State University, MICHELLE JOHANNES, Naval Research Laboratory — Layered mixed-metal oxides with different compositions of (Ni,Co,Mn) [NCM] or (Ni,Co,Al) [NCA] have been used in commercial lithium-ion batteries. Yet their defect physics and chemistry is still not well understood, despite having important implications for the electrochemical performance. In this presentation, we report a hybrid density functional study of intrinsic point defects in the compositions $\text{LiNi}_{1/3}\text{Co}_{1/3}\text{Mn}_{1/3}\text{O}_2$ ($\text{NCM}_{1/3}$) and $\text{LiNi}_{1/3}\text{Co}_{1/3}\text{Al}_{1/3}\text{O}_2$ ($\text{NCA}_{1/3}$) which can also be regarded as model compounds for NCM and NCA. We will discuss defect landscapes in $\text{NCM}_{1/3}$ and $\text{NCA}_{1/3}$ under relevant synthesis conditions with a focus on the formation of metal antisite defects and its implications on the electrochemical properties and ultimately the design of NCM and NCA cathode materials.

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