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First-principles studies of native defects in olivine phosphates KHANG HOANG, George Mason University and Naval Research Laboratory, MICHELLE JOHANNES, Naval Research Laboratory — Olivine phosphates $LiMPO_4$ (M=Mn, Fe, Co, Ni) are promising candidates for rechargeable Li-ion battery electrodes because of their energy storage capacity and electrochemical and thermal stability. It is known that native defects have strong effects on the performance of olivine phosphates. Yet, the formation and migration of these defects are not fully understood, and we expect that once such understanding has been established, one can envisage a solution for improving the materials' performance. In this talk, we present our first-principles density-functional theory studies of native point defects and defect complexes in $LiMPO_4$, and discuss the implications of these defects on the performance of the materials. Our results also provide guidelines for obtaining different native defects in experiments.

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