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Polaron formation and transport in olivine cathode materials MICHELLE JOHANNES, Naval Research Laboratory, KHANG HOANG, Naval Research Laboratory; George Mason University — One of the critical factors limiting Li ion battery performance is electronic conduction through the cathode material. In the olivine structure type materials, such as $LiFePO_4$, the parent materials are insulators with a gap of approximately 4 (or more) eV. The withdrawal of an electron results not in a band-type hole state, but rather a localized polaronic state. Transport then occurs via hopping of the polaron through the crystal. The measured electronic conduction in olivine materials depends on the transition metal cation type. In this study, we use density functional theory to compare formation of polarons in olivine materials with different transition metal cations: Mn, Fe, Co, and Ni. We show that the underlying electronic structure of the fully lithiated material (or fully delithiated material) essentially determines whether or not polaron formation is possible in localized *d*-states or whether the holes that result from adding or removing an electron reside in oxygen-derived states. We also investigate the facility of polaronic hopping by calculating the barrier between adjacent polaron sites in each of the four materials.

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