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Competing stability of inverse and normal spinel structures for lithium battery cathodes JISHNU BHATTACHARYA, CHRISTOPHER WOLVERTON, Northwestern University — Transition metal oxides comprise of an important class of cathode materials in rechargeable lithium ion batteries. Many of these materials occur in the spinel crystal structure, in which metal atoms are present in octahedral and tetrahedral interstices of a close-packed oxygen sublattice. Depending on whether the Li or the transition metal ions are found in the tetrahedral sites, one can form either the "normal" or "inverse" spinel structures. In the present study, we calculate from first principles the relative stability of the inverse vs. normal spinel for a series of transition metal oxides both at lithiated and delithiated limits. We find trends in the stability of the normal vs. inverse spinel are a strong function of lithium content, and explain these results in terms of the preference for metal/Li tetrahedral/octahedral coordination. Despite the similarities between these two structures, they can have a profound effect on the Li diffusivity. We also use our framework to address the stability of multicomponent inverse spinel electrodes, such as $LiNiVO_4$.

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