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Extracting the LiV3O8 Phase diagram by cluster expansion[1]
TONGHU JIANG, MICHAEL FALK, Department of Materials Science and Engineering, Johns Hopkins University — LiV3O8 as a lithium battery cathode material has many advantages over current commercialized counterparts, which has prompted interest in improving its electrochemical behavior. However, no clear picture of its structural chemistry and phase behavior has emerged from experimental investigations. In the current work, LiV3O8 was studied using computational methods. A cluster expansion was constructed based on energetic data from density functional theory calculation. The CE was employed to reveal structural information regarding this material. DFT calculation using the local density approximation were found to be deficient in correctly predicting ground states leading to mismatch between experimental and computational results, while generalized gradient approximation gives closer agreement with experimental data. A tentative phase diagram was obtained with the help of Metropolis Monte Carlo calculations.

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