Vacancy-driven anisotropic defect distribution in LiFePO$_4$\textsuperscript{1} JAEEK-WANG LEE, WU ZHOU, JUAN CARLOS IDROBO, Department of Physics and Astronomy, Vanderbilt University, Nashville, STEPHEN PENNYCOOK, Materials Science & Technology Division, Oak Ridge National Laboratory Oak Ridge, SOKRATES PANTELIDES, Department of Physics and Astronomy, Vanderbilt University, Nashville — It has been reported that iron cations occupying Li sites (Fe$_{Li}$) in LiFePO$_4$ are locally aggregated rather than homogeneously distributed in the lattice.\textsuperscript{1} Here we report a combination of density-functional calculations, statistical mechanics, electron-energy-loss spectra (EELS) and show the following. There is a strong binding energy between Fe$_{Li}$ and a lithium vacancy (V$_{Li}$), leading to clustering of Fe$_{Li}$ along the b-axis, as observed, corresponding to the shortest separation of the Fe$_{Li}$-V$_{Li}$ pair. EELS data find that a small fraction of Fe atoms are Fe$^{3+}$, which can be accounted for in terms V$_{Li}$-Fe$_{Li}$-V$_{Li}$ clusters formed along the b-axis.

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