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Vacancy-driven anisotropic defect distribution in $LiFePO_4$[1] JAEKWANG 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.[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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