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Insolubility of intercalants in strongly correlated oxides and phosphates ERIC ISAACS, CHRIS MARIANETTI, Department of Applied Physics and Applied Mathematics, Columbia University — Olivine lithium iron phosphate (Li_xFePO_4), a cathode material for Li-ion batteries, phase separates into the fully lithiated and fully delithiated phases according to experiment. Previous electronic structure calculations showed that while this phase separation is not predicted by DFT, it is captured by DFT+U due to the improved treatment of electronic correlations [F. Zhou et al., Phys. Rev. B 69, 201101 (2004).]. In order to understand the role of electronic correlations in phase separation, here we investigate the phase stability of Li_xFePO_4 and other strongly correlated oxide and phosphate intercalation compounds within DFT+U and DFT+DMFT. We present the relationship between computed formation energies and the on-site Coulomb repulsion and double-counting correction across different systems. In addition, we perform p-d model calculations in order to understand the mechanism at a minimal level.

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