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Impact of strong electronic correlations on the phase stability of oxide and phosphate intercalation materials ERIC ISAACS, CHRIS MARIANETTI, Department of Applied Physics and Applied Mathematics, Columbia University — Li intercalation in certain battery cathode materials such as Li_xFePO_4 (LFP) occurs via a two-phase (phase separated) process, which significantly impacts the voltage profile and charge/discharge kinetics. The phase separation in LFP is not predicted by density functional theory (DFT), but it is captured by DFT plus Hubbard U (DFT+U) suggesting the significant role of electronic correlations in determining its thermodynamic properties [F. Zhou et al., Phys. Rev. B 69, 201101 (2004).]. In order to understand the impact of such correlations on the phase stability of transition metal oxide and phosphate intercalation materials, here we investigate the formation energies of phase separating LFP, phase stable Li_xCoO_2, and phase stable $Sr_xLa_{1-x}TiO_3$ within DFT+U. We present the relationship between different formation energy contributions and the on-site Coulomb energy. Furthermore, we illustrate how band filling, *p-d* hybridization, magnetism, and charge and orbital ordering can impact the phase stability of such systems.

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