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Phase transformation and electronic structure characterization of Li_xFePO_4 by ab-initio calculations and soft x-ray spectroscopy YUNG JUI WANG, Northeastern Univ. (NU) and ALS, LBNL, B. BARBIELLINI, NU, XIAOSONG LIU, RUIMIN QIAO, ALS, LBNL, B. MORITZ, T. P. DEVEREAUX, Stanford Univ. and SLAC, HSIN LIN, National Univ. of Singapore, Singapore, ZAHID HUSSAIN, WANLI YANG, ALS, LBNL, A. BANSIL, NU — Olivine-structured Li_xFePO_4 with appropriate surface treatment is a battery cathode material with promising capacity, cost and safety specifications. Fe-L and O-K edge soft x-ray absorption and emission spectra directly probe the unoccupied and occupied electronic states in the vicinity the Fermi energy. We present a first principles calculation and a comparison with the spectra to investigate the electronic states of Li_xFePO_4. Upon fully (de)lithiation, the redistributed unoccupied Fe-3d and O-2p states indicate the fingerprints of the two-phase transformation. The redox couple is pinned such that a single electron injection into the valence states is well separated from the top of O-2p valence states due to Coulomb repulsion. We further explore the surface properties and discuss their implications on the performance and optimization of Li_xFePO_4. Work supported by the US DOE.

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