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Why $LiFePO_4$ is a safe battery electrode: Coulomb repulsion induced electron-state reshuffling upon lithiation YUNG JUI WANG, Northeastern Univ. (NU) and ALS, LBNL, XIAOSONG LIU, ALS, LBNL, B. BARBIELLINI, HASNAIN HAFIZ, SUSMITA BASAK, NU, JUN LIU, THOMAS RICHARDSON, EETD, LBNL, GUOJIUN SHU, FANGCHENG CHOU, National Taiwan Univ., TSU-CHIEN WENG, DENNIS NORDLUND, DIMOSTHENIS SOKARAS, SLAC, B. MORITZ, T. P. DEVEREAUX, Stanford Univ. and SLAC, RUIMIN QIAO, YI-DE CHUANG, ALS, LBNL, ARUN BANSIL, NU, ZAHID HUSSAIN, WANLI YANG, ALS, LBNL — We performed systematic experimental and theoretical studies based on soft X-ray emission, absorption, and hard X-ray Raman spectroscopy of Li_xFePO_4. The results show a non-rigid electron-state reconfiguration of both the occupied and unoccupied Fe-3d and O-2p states during the (de)lithiation process. The critical 3d electron state configurations are consistent with the calculations based on MBJGGA+U framework, which improves the overall lineshape prediction compared with the conventionally used GGA+U method. The combined experimental and theoretical studies show that the non-rigid electron state reshuffling guarantees the stability of oxygen during the redox reaction throughout the charge and discharge process of $LiFePO_4$ electrodes, leading to the intrinsic safe performance of the electrodes. Work supported by the US DOE.

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