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Visualizing redox orbitals and their potentials in olivine materials for advanced lithium-ion batteries HASNAIN HAFIZ, Northeastern Univ., K. SUZUKI, Gunma Univ., B. BARBIELLINI, Northeastern Univ., Y. ORIKASA, Ritsumeikan Univ., V. CALLEWAERT, Univ. Antwerpen, S. KAPRZYK, Northeastern Univ. and AGH U. of Sc. and Tech., M. ITOU, J.A.S.R.I., K. YAMAMOTO, Kyoto Univ., R. YAMADA, Gunma Univ., Y. UCHIMOTO, Kyoto Univ., Y. SAKURAI, J.A.S.R.I., H. SAKURAI, Gunma Univ. , A. BANSIL, Northeastern Univ. — The key reactions that take place in lithium batteries are reduction-oxidation (redox) reactions, which involve transfer of conduction electrons from the lithium anode to an orbital of the cathode. Our study of high-energy x-ray Compton scattering spectroscopy on olivine lithium iron phosphate ($LiFePO_4$) shows that inelastic scattering spectra of high-energy photons yield faithful reconstructions of the redox orbitals. The knowledge of the redox orbital-momentum distribution allows the extraction of information related to kinetic energies involved in the redox reactions and the visualization of trends in the voltage. Our results demonstrate that x-ray Compton scattering spectroscopy provides unique descriptors for monitoring fundamental quantum mechanical effects determining the battery voltage in olivine materials.

Hasnain Hafiz
Northeastern University

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