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Extracting the Redox Orbitals in Li Battery Materials with High-Resolution X-Ray Compton Scattering Spectroscopy B. BARBIELLINI, Northeastern U. (NU), K. SUZUKI, Gunma U., Y. ORIKASA, Kyoto U., N. GO, H. SAKURAI, Gunma U., S. KAPRZYK, AGH Krakaw and NU, M. ITOU, Spring-8 Japan, K. YAMAMOTO, Y. UCHIMOTO, Kyoto U., YUNG JUI WANG, NU and ALS Berkeley, H. HAFIZ, A. BANSIL, NU, Y. SAKURAI, Spring-8 Japan — We present an incisive spectroscopic technique for directly probing redox orbitals based on bulk electron momentum density measurements via high-resolution X-ray Compton scattering. Application of our method to spinel LixMn2O4 (a lithium ion battery cathode material) is discussed. The orbital involved in lithium insertion and extraction process is mainly the oxygen 2p orbital. Moreover, the manganese 3d states are shown to experience spatial delocalization involving 0.16 electrons per Mn site during the battery operation. Our analysis provides a clear understanding of the fundamental redox process involved in the working of the lithium ion battery. Work supported in part by the US DOE.

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