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Identifying a descriptor for d-orbital delocalization in cathodes of Li batteries based on x-ray Compton scattering B. BARBIELLINI, Northeastern U., K. SUZUKI , Gunma U., Y. ORIKASA , Kyoto U., S. KAPRZYK, Northeastern U. and AGH U. of Sc. and Tech., M. ITOU , JASRI SPring-8, K. YAMAMOTO, Kyoto U., YUNG JUI WANG, H. HAFIZ, Northeastern U., R. YAMADA , Gunma U., Y. UCHIMOTO, Kyoto U., A. BANSIL, Northeastern U., Y. SAKURAI, JASRI SPring-8, H. SAKURAI, Gunma U. — We discuss how x-ray Compton scattering spectra can be used for investigating the evolution of electronic states in cathode materials of Li batteries under the lithiation/delithiation process. In particular, our analysis of the Compton spectra taken from polycrystalline Li_xCoO_2 samples shows that the spectra are dominated by the contribution of the O $2p$ redox orbital. We identify a distinct signature of Co $3d$ orbital delocalization, which is tied directly to the conductivity of the material, providing a descriptor [1] based on Compton spectra for monitoring the lithiation range with improved conductivity and kinetics for electrochemical operation. Our study demonstrates that Compton scattering spectroscopy can provide a window for probing complex electronic mechanisms underlying the charging and discharging processes in Li-battery materials.

[1] B. Barbiellini *et al.* Applied Physics Letters **109** , 073102 (2016)

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