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Redox orbital and electronic structure in energy materials by Compton scattering spectroscopy

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Compton scattering is one of the powerful tool for investigating electronic structure of the materials. Advantage of this technique is that Compton scattering use high-energy X-rays over 100 keV, which enables bulk sensitive measurement. Furthermore, Compton profile obtained from this technique reflects occupied orbitals of electrons upon Li insertion. We have applied this technique to electrode materials used for Li-ion battery, especially $Li_xMn_2O_4$ and Li_xCoO_2. The Compton scattering experiments were performed on the BL08W beamline at the SPring-8 synchrotron facility in Japan. Results of our Compton profile measurement show an increment of itinerant electrons with Li insertion in both materials. By comparing experiment with first-principles calculations, we deduce that this increase of itinerant electrons has O 2p character. On the other hand, 3d orbitals of transition metals become less localized at the range of Li concentration corresponding to the optimal battery performance both for the $Li_xMn_2O_4$ and Li_xCoO_2 cathodes. This 3d orbitals delocalization effect is associated with electron conductivity properties. Therefore, Compton scattering spectroscopy can provide new descriptors for electrode conductivity.

Biography

Kosuke Suzuki has completed his PhD at Gunma University. His interest includes “Electronic structure of energy materials and Compton scattering technique”. He has published 29 papers in journals, proceedings and reports.

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