Poster Presentation

MS106.P02

Redox orbitals in LixMn2O4 (0<x<2) studied by X-ray Compton scattering

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LixMn2O4 is attracting much interest as a positive electrode material for Li-ion rechargeable batteries. Redox orbitals of LixMn2O4 under the charge or discharge process are not fully understood yet. Some band calculations have pointed out that intercalated Li 2s electrons occupy Mn sites or down-spin Mn 3d bands [1,2]. On the other hand molecular orbital calculation has reported the Li 2s electrons occupy O sites [3]. To clarify the redox orbital is important to understand the electrochemical reaction in the electrodes. In this study we have investigated the redox orbitals in LixMn2O4 by X-ray Compton scattering. Compton profiles were measured at BL08W of SPring-8, Japan. The energy of incident X-rays were 115keV and the scattering angle was 165 degrees. Energy spectra of Compton scattered X-rays were measured using a two-dimensional position sensitive detector. The measurements were performed under room temperature and vacuum conditions. Samples are polycrystalline of LixMn2O4 (x=0.5, 1.1, 1.2, 1.8 and 2.0). In order to clarify the redox orbitals of LixMn2O4, we obtained difference Compton profiles which represent the incremental electronic states on Li intercalation. Comparing the results with KKR-CPA and DFT calculations, we found that the O 2p bands play an important role for the redox process in LixMn2O4 with 0<x<2.

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Keywords: Compton profile, redox orbital, Li-ion battery