Abstract Submitted
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Electronic structure of Na_xCoO_2 investigated by X-ray absorption spectroscopy with Ab initio calculation[1] PAO-AN LIN, JIUNN-YUAN LIN, BEN HSU, HORNG -TAY JENG, CHEN-SHIUNG HSUE, YIA-CHUNG CHANG — The soft X-ray absorption spectra (XAS) of Na_xCoO_2 revealed marked and puzzling polarization dependence. It can not be explained by the degeneracy of e_g states generally believed in Na_xCoO_2. We fabricated the thin films of x = 0.68 and x = 0.75 to investigate the polarization dependence of XAS. Within the first principles DFT calculations, we have explanations for this phenomenon. After the analysis of the DOS of Na_xCoO_2, we presume that the pre-edge peaks at 529 eV and 530 eV of Na_xCoO_2 O-K edge may be not solely due to the unoccupied states of Co3+ and Co4+ eg states, but also due to the spacial asymmetry in the occupied Co 3d orbitals. Due to the hybridization between Co 3d & O 2p orbitals, the $p_{x,y}$ and p_z states will be non-degenerate.

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