

Abstract Submitted  
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**Theoretical and Experimental Co *K*-edge XAS of Layered Cobalt Oxides Catalysts**<sup>1</sup> MICHAL BAJDICH, Joint Center for Artificial Photosynthesis, LBL, CA, DANIEL FRIEBEL, SLAC National Accelerator Laboratory, CA, JCAP, BOON S. YEO, Dept. of Chem. and Bio. Eng., UCB, CA, MARY LOUIE, JCAP, UCB, DANIEL J. MILLER, SLAC, HERNAN S. CASALONGUE, SLAC, JCAP, FELIX MBUGA, Stanford U., CA, TSU-CHIEN WENG, DENNIS NORDLUND, DIMOSTHENES SOKARAS, SLAC, ALEXIS T. BELL, JCAP, UCB, ANDERS NILSSON, SLAC, JCAP — The efficient water oxidation for fuel production from sunlight, with the use of earth-abundant catalysts, is of high importance to photo-fuel cell research. Recent experimental investigations of Co-oxide based catalysts under active conditions of water oxidation show evidence for layered cobalt-oxide structures with possible cation intercalation from electrolyte. To gain insight into our experimentally measured Co *K*-edge x-ray absorption spectra of Co-oxide anodes compared to spectra of powder standards such as CoOOH, Co(OH)<sub>2</sub> and Co<sub>3</sub>3O<sub>4</sub>, we perform theoretical investigations of these spectra. We employ density functional theory plus U (DFT+U) calculations of *K*-edge x-ray absorption spectra using core-hole approach which has been shown to accurately capture the pre-edge features of similar  $\alpha$ -LiCoO<sub>2</sub> [1]. We consider  $\beta$ -CoOOH,  $\alpha$ -KCoO<sub>2</sub>,  $\gamma$ -K<sub>0.5</sub>CoO<sub>2</sub> structures as possible candidates.

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Michal Bajdich  
Joint Center for Artificial Photosynthesis, LBL, CA

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