

Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

X-ray absorption spectroscopy of lithium sulfur battery reaction intermediates KEVIN WUJCIK, Dept. of Chemical and Biomolecular Engineering, University of California, Berkeley, TOD PASCAL, DAVID PRENDERGAST, Molecular Foundry, Lawrence Berkeley National Laboratory, NITASH BALSARA, Dept. of Chemical and Biomolecular Engineering, University of California, Berkeley — Lithium sulfur batteries have a theoretical energy density nearly five times greater than current lithium ion battery standards, but questions still remain regarding the reaction pathways through which soluble lithium polysulfide (Li_2S_x , “x” ranging from 2 to 8) reaction intermediates are formed. Complicating spectro-electrochemical approaches to elucidate redox pathways is the challenge of obtaining spectral standards for individual Li_2S_x species. Lithium polysulfides cannot be isolated as individual component and exist only in solution as a distribution of different Li_2S_x molecules formed via disproportionation reactions (e.g. $2\text{Li}_2\text{S}_4$ goes to $\text{Li}_2\text{S}_3 + \text{Li}_2\text{S}_5$). X-ray absorption spectroscopy (XAS) at the sulfur K-edge has recently been employed as a technique to study Li-S chemistry. We have recently obtained XAS standards for individual Li_2S_x species via first principles DFT simulations and the excited electron and core hole approach. Here, experimental sulfur K-edge XAS of Li_2S_x species dissolved in poly(ethylene oxide) are compared to spectra obtained from analogous theoretical calculations. The impact that polysulfide solution concentration and the presence of other lithium salts (e.g. LiNO_3) have on X-ray spectra of Li_2S_x species is explored via experiment and theory.

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Date submitted: 14 Nov 2014

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