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X-ray absorption spectroscopy of reaction intermediates of lithium-sulfur batteries dissolved in polymer electrolytes KEVIN WUJCIK, NITASH BALSARA, University of California, Berkeley — Lithium polysulfide reaction intermediates formed during the charge and discharge reactions of a lithium-sulfur battery are known to diffuse out of the cathode during cycling, thus lowering battery capacity and lifetime. While numerous techniques have been developed to confine intermediates to the battery cathode, little is known about the complex reaction mechanism responsible for their formation. Work to understand the reaction mechanism requires an experimental technique capable of distinguishing the various lithium polysulfide intermediates formed during the charge/discharge reactions. We report on the use of x-ray absorption spectroscopy (XAS) to distinguish lithium polysulfide molecules in polymer electrolytes. Polysulfide intermediates dissolved in poly(ethylene oxide) and a block copolymer of polystyrene-poly(ethylene oxide) were probed at the oxygen, carbon, and sulfur K-edges. Simulated x-ray spectra based on ab-initio molecular dynamics were used to interpret experimental x-ray spectra. Theories regarding the physical and chemical nature of the polysulfide–polymer electrolyte interaction were developed.

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