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X-ray absorption spectroscopy as a probe of dissolved polysulfides in lithium sulfur batteries TOD PASCAL, DAVID PRENDERGAST, Lawrence Berkeley National Lab — There has been enormous interest lately in lithium sulfur batteries, since they have 5 times the theoretical capacity of lithium ion batteries. Large-scale adoption of this technology has been hampered by numerous shortcomings, chiefly the poor utilization of the active cathode material and rapid capacity fading during cycling. Overcoming these limitations requires methods capable of identifying and quantifying the products of the poorly understood electrochemical reactions. One recent advance has been the use of X-ray absorption spectroscopy (XAS), an element-specific probe of the unoccupied energy levels around an excited atom upon absorption of an X-ray photon, to identify the reaction products and intermediates. In this talk, we'll present first principles molecular dynamics and spectral simulations of dissolved lithium polysulfide species, showing how finite temperature dynamics, molecular geometry, molecular charge state and solvent environment conspire to determine the peak positions and intensity of the XAS. We'll present a spectral analysis of the radical (-1e charge) species, and reveal a unique low energy feature that can be used to identify these species from their more common dianion (-2e charge) counterparts.

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