Supporting Information: Discharge Mechanism in a Solid-State Lithium-Sulfur Cell by Operando X-ray Absorption Spectroscopy

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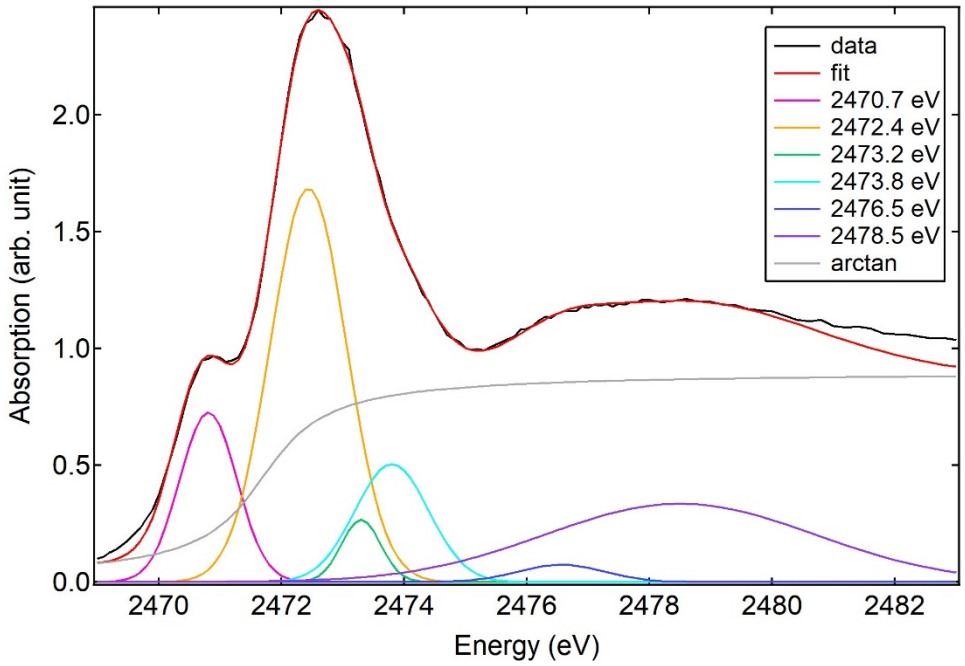

Figure S1. Example of fitting a discharge XAS spectra (175 mAh/g depth of discharge) with 6 gaussian peaks and a step function: 1 gaussian centered at 2470.7 eV for the pre-edge peak, 2 gaussians centered at 2472.4 eV and 2473.2 eV for the main-edge peak, 1 gaussian centered at 2473.8 eV, 1 gaussian centered at 2476.5 eV, and 1 gaussian centered at 2478.5 eV.

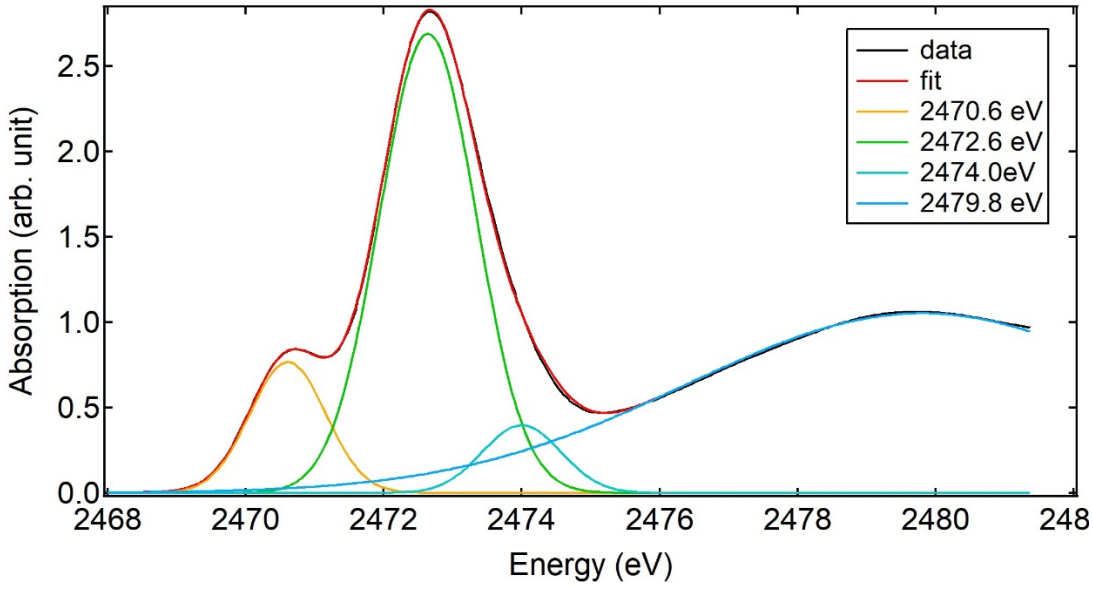

Figure S2. Example of fitting a theoretical XAS spectra (Li_2S_6) with 1 gaussian peak centered at 2470.6 eV for the pre-edge peak and 2 gaussian peaks centered at 2472.6 eV and 2474.00 eV for the main-edge peak

Note that equation (8) differs slightly from our previous work.[1] The fitting procedure used in the present paper used two gaussian peaks instead of one to fit the main-edge peak. This is to account for the asymmetry of the main-edge peak.

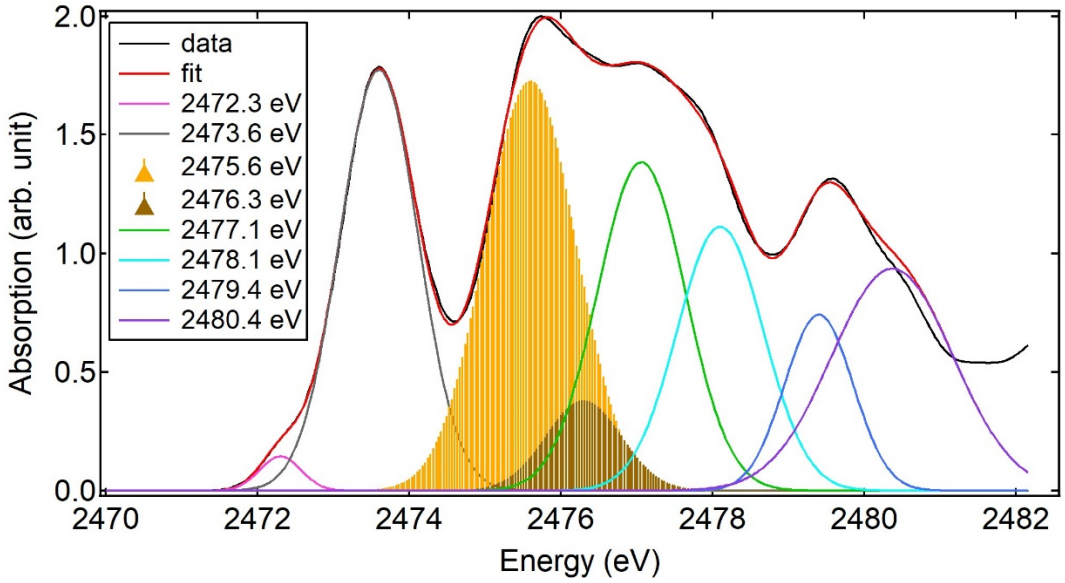

Figure S3. Fitting Li_2S theoretical XAS spectrum with 10 gaussian peaks centered at 2472.3 eV, 2473.6 eV, 2475.6 eV, 2476.3 eV, 2477.1 eV, 2478.1 eV, 2479.4 eV, and 2480.4 eV. The sum of the shaded areas under peaks centered at 2475.6 eV and 2476.3 eV is A_s^{Th}.

Reference:

1. Wujcik, K. H., Wang, D. R., Pascal, T. A., Prendergast, D. & Balsara, N. P. In Situ X-ray Absorption Spectroscopy Studies of Discharge Reactions in a Thick Cathode of a Lithium Sulfur Battery. *J. Electrochem. Soc.* **164,** A18–A27 (2017).