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Nanoscale electrochemical conversion in post-lithium-ion batteries tracked by operando scattering and stochastic modelling

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Realizing post-lithium-ion batteries, such as Metal-sulfur (Li-S) and metal-air (Li-O2) batteries, could be game-changing due to theoretical specific capacity amongst the highest of all batteries paired with the low cost and sustainability of the active materials. However, the insufficient understanding of the mechanism that reversibly converts the active materials between their lithiated and de-lithiated state slows down the practical realization.

In this talk, I will present the results of employing operando small and wide angle X-ray scattering (SAXS/WAXS) and operando small angle neutron scattering (SANS) to track the growth and dissolution of solid deposits from atomic to sub-micron scales during operating a Li-S battery cell [1]. Machine-learning-assisted stochastic modelling based on the SANS (and SAXS) data allows quantification of the chemical phase evolution during discharge and charge. Combined with complementary data from transmission electron microscopy and Raman spectroscopy, we show that the deposit is comprised of nanocrystalline Li2S and smaller, solid short-chain polysulfide particles. Knowing this has important implications for influencing the reaction mechanism. As a second example, I will show results from operando SAXS/WAXS on Li-O2 battery cathodes, tracking the reversible formation and dissolution of Li2O2 on the nanoscale [2, 3].

The examples on Li-S and Li-O2 batteries demonstrate that structural information on mesoscopic length scales is key to understanding complex transformations in energy materials. Operando SAXS/SANS, (cryo-) electron microscopy, and machine-learning-assisted stochastic modelling combine the advantages of integral time-resolved structural information, local element-specific microscopy, and quantitative data analysis.

References:

[1] C. Prehal, V. Wood et al. Nature Communications 13, 6326 (2022)

[2] C. Prehal, S.A. Freunberger et al. PNAS 118, 14, e2021893118 (2021)

[3] C. Prehal, S.A. Freunberger et al. ACS Energy Letters 7, 9, 3112 (2022)

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