Tackling complexity in post-Li-ion battery research: from machine learning-assisted scattering to data-driven experimental design

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Post-lithium-ion batteries such as lithium-sulfur (Li-S) and sodium-ion (Na-ion) promise higher energy density and more sustainable raw materials. However, their key processes, from conversion reactions and nanoscale phase transformations to complex, multi-parameter synthesis routes, remain fundamentally hard to understand. In this talk, I discuss how machine learning tackles this complexity by (i) interpreting information-rich, structurally complex operando data of Li-S batteries, and (ii) navigating high-dimensional experimental parameter spaces using active learning for optimizing Na-ion battery anodes.

In the first part, I show how operando SAXS/WAXS and SANS, combined with machine learning-accelerated stochastic modelling, quantify nanoscale conversion mechanisms across solid-liquid-solid and quasi-solid-state pathways in Li-S batteries [1-3]. Experiments were performed at ELETTRA (AustroSAXS), our own lab facilities and at ILL (D22). Combined with cryo-TEM, the data reveal a biphasic deposit of nanocrystalline Li_2S and amorphous short-chain polysulfide. Resolving this detail across the full state-of-charge range only became practical using neural-network-based data fitting.

In the second part, I turn to active learning for navigating large parameter spaces in battery materials synthesis and testing [4]. Bayesian optimization with Gaussian process surrogate models automatically selects the next most informative experiment, reducing the measurements needed to identify optimal conditions. I present work applying this approach to scattering-based quality control of hard carbon anode synthesis for Na-ion batteries, where active learning links structural descriptors (from SAXS) to sodium storage performance.

References:

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Short bio:

Christian Prehal is Assistant Professor and Head of the Energy Materials Lab at the Department of Chemistry and Physics of Materials at the University of Salzburg, Austria. His team develops operando X-ray/neutron scattering and cryo-TEM methods, combined with machine learning, to study electrochemical conversion mechanisms in lithium-sulfur and sodium-ion batteries. After a PhD at Montanuniversität Leoben, he was a postdoc at TU Graz (Freunberger group) and ETH Zürich (Vanessa Wood group, Marie-Curie fellow) before starting his lab in Salzburg in 2023, funded by an ERC Starting Grant (SOLIDCON).