Contribution ID: **98** Type: **Invited**

Dynamic surfaces and interfaces in batteries

Tuesday, 16 July 2024 16:20 (30 minutes)

Dynamic surfaces and interfaces in batteries

Understanding the dynamic properties of surfaces and interfaces is foundational to many scientific disciplines. In electrochemistry, charge transfer occurs at the solid–liquid interface between electrode and electrolyte. For almost all systems and under most conditions, these interfaces are dynamic and evolve with time. This is particularly prominent for the surface electrochemistry in ion batteries because these are operated outside the electrochemical stability window of typical aprotic electrolytes leading to the formation and evolution of the so-called solid electrolyte interphase (SEI) [1,2]. Via its electron-blocking and ion-conduction properties, the SEI governs battery cell lifetime and kinetics [1].

In the first part of the talk, the particular usefulness of X-ray methods for studying electrochemical systems in general and the surface electrochemistry of ion batteries in particular will be introduced. I.e., X-ray methods can be performed in operando modality, and they provide quantitative information on an absolute scale ("X-ray Coulomb counting").

The second part of the talk will focus on several examples in which we utilized surface X-ray scattering to understand the surface electrochemistry of ion batteries using model electrodes. The examples include the growth and evolution of the SEI on Si anodes and the respective correlation between SEI structure and electrochemical performance [3]. Moreover, the origin of LiF in the SEI will be addressed. Towards this end, we sought out a multimodal operando (synchrotron X-ray-based) experimental and theoretical approach [4]. Our results reveal that LiF nucleates via the electrocatalytic reduction of HF followed by significant PF6- anion reduction. Furthermore, X-ray chemistry-X-ray probe experiments of super-concentrated "water-in-salt" electrolytes will be discussed, in which we observed interfacial speciation-dependent surface-reduction of anions [5].

The final part of the talk will be devoted to future science-driven opportunities for surface X-ray scattering at DLRs and XFELs under the mottos "Surface X-ray scattering goes fast", "Surface X-ray scattering goes ultrafast", and "Surface X-ray scattering goes small".

[1] Xu, J. Power Sources 559, 232652 (2023)
[2] Cao, Steinrück, Molecular-scale synchrotron X-ray investigations of solid-liquid interfaces in lithium-ion batteries, Encyclopedia of Solid-Liquid Interfaces (2024)
[3] Cao et al., Acc. Chem. Res. 52, 2673-2683 (2019)
[4] Cao et al., Chem. Mater. 33, 7315-7336 (2021
[5] Steinrück et al., Angew. Chem. Int. Ed. 59, 23180-23187 (2020)

Please select the related topic from the list below

Dynamics of surfaces, interfaces, and nanostructures

Primary author: STEINRÜCK, Hans-Georg (Forschungszentrum Jülich, INW & RWTH Aachen)

Presenter: STEINRÜCK, Hans-Georg (Forschungszentrum Jülich, INW & RWTH Aachen)

Session Classification: Dynamics of surfaces, interfaces, and nanostructures