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In situ x-ray diffraction studies of the atomic structure and charge distribution at the electrochemical interface

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The presence of specifically adsorbed anions can significantly affect the electrochemical reactivity of a metal electrode which is of major interest for galvanic deposition, etching, corrosion and electrocatalysis. In-situ surface x-ray diffraction has enabled an atomic/molecular-level understanding of the interface under reactive conditions, including its potential and time dependence, to be developed. While information about the atomic structure of the electrode surface in electrochemical in-situ cells has been widely investigated, insight into the charge distribution and the structure of the electrolyte at the interface is still lacking. Advances in these directions offer possibilities in elucidating atomic scale models of the electrochemical interface and thus will help to establish structure-stability-reactivity relationships.
A fundamental understanding of the nature of the charge transfer, especially the influence of the applied potential and the screening by the electrolyte, is a major goal in electrochemistry to better understand electrochemical processes and charge transfer during adsorption and deposition. [1]
Thus combining x-ray spectroscopy and x-ray diffraction to gain site specific information about the charge distribution at buried interfaces is a promising tool. [2,3]

Examples of how the use of surface x-ray scattering techniques can help to characterise electrochemical interfaces in-situ in order to link, structure, reactivity and stability will be presented. [4-5] Advances in these directions offer possibilities in elucidating atomic scale models of the electrochemical interface and thus will help to establish structure-stability-reactivity relationships and to understand growth kinetics and electrochemical phase formation.

References:

[1] Y. Gründer and C. A. Lucas, Nano Energy 29, 378 (2016).
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[4] Y. Grunder et al., Charge Reorganization at the Adsorbate Covered Electrode Surface Probed through in Situ Resonant X-ray Diffraction Combined with ab Initio Modeling; Phys. Chem. C 2022, 126, 9, 4612–4619
[5] Yvonne Soldo-Olivier et al., Unraveling the Charge Distribution at the Metal-Electrolyte Interface Coupling in Situ Surface Resonant X-Ray Diffraction with Ab Initio Calculations, ACS Catal. 2022, 12, 4, 2375–2380

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Interfaces during chemical reactions and catalysis

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