

# In situ studies of the atomic structure/charge distribution at the electrochemical interface

**Yvonne Grunder**

Oliver Lodge Laboratory, Department of Physics,

University of Liverpool, Liverpool L69 7ZE, UK

Email: grunder@liverpool.ac.uk

Electrochemical interfaces play a crucial role in many systems used for clean energy production, conversion and storage. Improving fundamental understanding of the electrochemical interface will thus help to solve current problems in these systems, e.g. the stability of the electrode and electrolyte and the charge transfer mechanism.

*In-situ* x-ray characterisation techniques have enabled an atomic/molecular-level understanding of the interface [1] 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 by *in-situ* surface x-ray characterisation, 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. [2]

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. [3,4]

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.

## References:

[1] B. Baggio, Y. Grunder, *Annu. Rev. Anal. Chem.*, **2021**, 14, 12.1-12.21.

[2] Y. Gründer *et al.*, *J. Phys. Chem. C*, **2012**, 116, 6283.

[3] Y. Gründer and C. A. Lucas, *Phys. Chem. Chem. Phys.*, **2017**, 19, 8416.

[4] Y. Joly *et al.*, *J. Chem. Theory Comput.*, **2018**, 14, 973-980.

[6] Y. Gründer, *et al.*, *Surface Sci.*, **2019**, 680, 113-118.