

Temporal Electronic and Structural Landscapes in Catalytic Water-Splitting

Simone Techert^{1,2}

1) Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany

2) Fakultät für Physik, Georg-August Universität, Göttingen, Germany

*Contact: simone.techert@desy.de

Keywords: water splitting, catalysis, time-resolved/ultrafast elastic and inelastic X-ray scattering, free-electron lasers, synchrotrons, liquid-jet technologies

Water splitting is a crucial process for hydrogen production, which is essential for the development of a sustainable energy economy. It enables the conversion of water into hydrogen and oxygen using renewable energy sources, providing an alternative to fossil fuels. As water is an abundant resource and the OH-water bond is one of the strongest chemical bonds in nature, water splitting, when fueled by renewable energy, becomes a sustainable and scalable method to unlock the full potential of renewable energy technologies.

In this talk, I will present our method developments for the years 2023-2025 and our new research studies on catalytic water splitting. This continues our efforts to understand and uncover the detailed atomistic mechanism of the oxygen evolution reaction (OER) 1-3. The methods of choice are high-resolution photon-in / photon-out experiments at high repetition x-ray sources (synchrotrons and FELs) - elastic and inelastic scattering studies, with special emphasis on resonant inelastic x-ray scattering (RIXS).

I will present our recent in-situ, operando or time-resolved soft X-ray studies exemplified by OER of different highly efficient catalysts of the types metal oxide-doped metal oxide systems (AO/BO) and - for comparison - ABO₃ (A, B = transition metals). These catalysts were selected because they are able to break the scaling law (i.e. they are more efficient than the standard systems interpolated in a thermodynamic model).

Since the inelastic soft X-ray spectroscopy studies are element and oxidation state selective, the presentation starts with different types of OER from the perspective of the catalyst (metal L-edges). Using polarization-dependent metal L-edge soft X-ray spectroscopy, we have investigated the catalyst intermediates formed during OER on ideally grown surfaces and compared them with those formed when nanoparticles are used. The results are discussed in the context of ultrafast RIXS studies of similar systems, but in a different context - ultrafast photoexcitation studies with a RIXS energy resolution of over 100 meV at the European XFEL 4.

Zooming into the Helmholtz layer by oxygen K-edge spectroscopy and maintaining the high RIXS energy resolution of 100 meV (and beyond), the water adsorption results are discussed in relation to the electrolysis active layers on the catalyst surface of the different catalysts listed above.

¹ S. S. Nair Lalithambika, ST et al. *Adv. En. Mat.* 2025, 2404280 (2025). DOI: 10.1002/aenm.202404280

² J. J. Velazquez-Garcia, ST et al., *Chem. Sci.* 15, 13531-13540 (2024). DOI: 10.1039/d4sc02933j

³ T. Reuss, ST et al., *Acc. Chem. Res.* 56, 203-214 (2023). DOI: 10.1021/acs.accounts.2c00525

⁴ J. Schlappa, S. S. Nair Lalithambika, ST, A. Scherz, A. Foehlich et al., *J. Syn. Rad.* 32, 29-45 (2025). DOI: 10.1107/S1600577524010890