# O 24: Overview Talk Yang Shao-Horn

Time: Tuesday 9:30–10:15 Location: S054

**Invited Talk** O 24.1 Tue 9:30 S054

**Oxygen Evolution on Rutile Ruthenium and Iridium Dioxides** — •Yang Shao-Horn — MIT, Cambridge, MA, USA

Rutile oxides have been studied intensively for water oxidation in acidic solutions. Unfortunately, atomic details of processes occurring at the electrified interface and active sites are not well understood. In this work, we combine in situ surface sensitive techniques, electrochemical mass spectrometry and density functional theory calculations to elucidate oxygen evolution reaction (OER) on ruthenium and iridium dioxides. Using synchrotron-based ambient pressure X-ray photoelectron spectroscopy and in situ surface diffraction on single crystal surfaces coupled with density functional theory calculations, we show that with increasing potential from 0.5 VRHE, adsorbed water on the coordinatively unsaturated sites (CUS) is successively deprotonated. Surface diffraction measurements and computation reveal what steps can be rate-limiting for OER. Such analyses are applied also to CUS sites on other surfaces as well as different IrO2 surfaces, from which fingerprints of surface oxygen atoms are correlated with OER activity. In order to connect learnings from single-crystals with practical catalysts, electrochemical activity measurements were combined with highly sensitive electrochemical mass spectrometry to quantify the amount of evolved oxygen and reveal three Tafel regimes at different overpotentials, which was rationalized by the coverage of the reaction intermediates. In summary, by employing different experimental and theoretical techniques to model surfaces and practical catalysts, we discuss the nature of the active sites catalyzing OER on ruthenium and iridium dioxides.