# O 56: Key Note IV

Time: Tuesday 15:30–16:00 Location: R1

**Plenary Talk** O 56.1 Tue 15:30 R1

**Meta-stable intermediates of OER catalysis: connecting their time-resolved spectra to thermodynamic descriptors** — •Tanja Cuk, Ilya Vinogradov, Aritra Mandal, Suryansh Singh, and Hanna Lyle — University of Colorado, Boulder, Boulder USA

The intermediate steps of catalytic mechanisms are challenging to identify experimentally, but are critical to understanding the speed, stability, and selectivity of product evolution. In the laboratory, we employ photo-triggered vibrational and electronic spectroscopy to time-resolve the catalytic cycle at a surface, identifying meta-stable intermediates and critical transition states which connect one to another. The focus is on the highly selective oxygen evolution reaction (OER) at the semiconductor (SrTiO3)-aqueous interface, triggered by an ultrafast light pulse in an electrochemical cell. A short summary of past work will be given, which resolved the structure and picosecond formation kinetics of the first meta-stable electron-transfer intermediates (Ti-OH*) of OER. The main topic will concern the recent results that connect the time-resolved kinetics to a thermodynamic free energy difference, (Delta G (OH*)), often used to differentiate the activity of materials. In particular, a Langmuir isotherm as a function of electrolyte pH extracts an effective equilibrium constant for this reaction step using a principal component analysis of the optical spectra. In so doing, reaction conditions that shift equilibria of separable catalytic steps become an important, independent axis to the time & energy axes of the spectroscopy.