Organization for Cultural Diversity in Science Seminar

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"Resolving a Catalytic Mechanism at an Electrode Surface with High Time-resolution: Experimental Identification of Theorical Descriptors"

Abstract: Catalytic mechanisms at electrode surfaces guide the development of electrochemically-controlled energy storing reactions and chemical synthesis. The intermediate steps of these mechanisms are challenging to identify experimentally, but are critical to understanding the speed, stability, and selectivity of product evolution. In my group, 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 water oxidation reaction at the semiconductor ($SrTiO_3$)-aqueous interface, triggered by an ultrafast light pulse in an electrochemical cell. Here, I will summarize the work done to date by the group: the structure and dynamics of the initial intermediates that trap charge (Ti-O^{*-} and Ti-O^{*+}-Ti) from their picosecond birth at the surface through the next event at microseconds, suggested to be the formation of the first O-O bond of O_2 evolution. There will be a focus on how time-resolving the intermediates leads to experimental identification of largely theoretical descriptors of oxygen evolution, such as the binding energy of the first meta-stable, electron-deficient oxygen intermediates (generally, M-OH^*). In so doing, reaction conditions that shift equilibria become an important, independent axis to the time & energy axes of the spectroscopy. While many open questions remain, these experiments provide and benchmark the opportunity to quantify intermediates at an electrode surface and follow a heterogeneous catalytic cycle in time

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4:00 p.m. | ZOOM

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More information