Theoretical and Physical Chemistry Institute
National Hellenic Research Foundation

Vass. Constantinou 48, Athens

ONLINE LECTURE

“Charge Transfer Mechanisms & Selectivity in Heterogeneous Electrocatalysis”

Dr. Vanessa J. Bukas

Theory Department,
Fritz-Haber-Institute of the Max-Planck-Society,
Berlin, Germany

Thursday, June 3, 2021, 12:00

Link: Click here to join the lecture

Passcode: 264591

Charge Transfer Mechanisms & Selectivity in Heterogeneous Electrocatalysis

Dr. Vanessa J. Bukas

Theory Department, Fritz-Haber-Institute of the Max-Planck-Society,
Faradayweg 4-6, 14195, Berlin, Germany

Heterogeneous electrocatalysis holds promise for the continued production of fuels and chemicals in a sustainable, fossil-free future. Despite substantial progress over the past decade, however, there is still an urgent need for improved electrocatalysts before clean energy technologies can be considered viable for widespread application. A key challenge in meeting this goal will be to better control catalyst selectivity, especially toward high-value products such as e.g., long hydrocarbons, oxygenates, and ammonia. Such efforts are presently hindered by our limited fundamental understanding of electrocatalytic selectivity in general. Even for extremely well-defined experimental systems, identity of the favored product is often unexplained and cannot be rationalized by popular thermodynamic models of coupled-proton electron transfers (PCETs) that currently define the state-of-the-art in computational electrocatalysis.

This talk will challenge prevalent mechanistic assumptions and explore microscopic reaction mechanisms under conditions of limiting electron or proton availability, as a means to selectively suppress specific PCET steps or reaction routes. The idea will be showcased for a handful of systems where delayed charge transfer is suggested as a determining factor to the resulting product selectivity. Atomistic models, based mainly on density functional theory, will further be used to show that such mechanisms can explain key experimental findings and even be exploited to systematically steer product selectivity in technologically important electrochemical processes. This suggests departure from the common-practice approach of predicting activity trends based on thermodynamic descriptors of specific charge-neutral surface intermediates and underlines interfacial charge transfer kinetics as a promising research direction that may help gain better control over electrocatalytic selectivity.