

Materials Engineering Program
Texas Center for Superconductivity at the University of Houston
Center for Integrated Bio and Nano Systems

Theoretical Studies of Activity-Stability-Selectivity Relations in Water-Splitting Electrocatalysts

April 5, 2024

Face to Face, 1:00 – 2:00 pm

Houston Science Center (HSC), Rm 102

Prof. Vitali Alexandrov
University of Nebraska–Lincoln



Abstract: The development of active, selective, and stable electrocatalysts is crucial for making a variety of electrochemical conversion reactions more efficient. Importantly, there are some fundamental relationships between these critical properties that we are trying to understand better. In this talk, I will discuss several examples from recent research in the area of oxygen electrocatalysis focusing on DFT-based simulations of activity, selectivity, and stability properties. First, I will present some results of our collaborative theory-experiment investigation of the influence of alkali metal cations on the oxygen reduction reaction activity over Pt-based alloys. Second, I will discuss recent computational studies highlighting the relationships between activity and selectivity of hydrogen peroxide production via the water oxidation reaction using metal-oxide and doped graphene-based catalysts. Third, I will also present our recent computational results on the relationship between the activity and stability of metal oxide-based oxygen evolution reaction electrocatalysts as a function of lattice strain.

Bio: Vitaly Alexandrov is Richard L. McNeel Associate Professor in the Department of Chemical and Biomolecular Engineering at the University of Nebraska-Lincoln (UNL). He studied electrochemistry (Diploma) and quantum chemistry (M.S.) at St. Petersburg State University and received his Ph.D. degree from Max Planck Institute for Solid State Research in 2009. He subsequently worked as a postdoctoral researcher at the University of California at Davis, the University of California at Berkeley, and the Pacific Northwest National Laboratory before joining UNL as an Assistant Professor in 2015. His research focuses on theoretical/computational studies of electrochemical materials with applications in energy conversion and storage. He is the recipient of NSF CAREER and ACS PRF awards and currently serves on the Editorial Advisory Board of the Journal of Physical Chemistry C.