

UNIVERSITY OF CALIFORNIA, IRVINE

# THE DEPARTMENT OF MATERIALS SCIENCE AND ENGINEERING



## Professor and Vice Chair Anastassia Alexandrova

Dept. of Chemistry and Biochemistry  
University of California, Los Angeles

Thursday, November 17, 2022

2:00-3:20 PM

Location: ISEB Building - Colloquium 1200

## Heterogeneous Catalysts Set In Motion By Reaction Conditions: Ensembles Of Metastable States Break The Rules Of Catalysis

**Abstract:** The talk will focus on heterogeneous (electro)catalytic interfaces that are exceptionally dynamic under reaction conditions. A prime example is supported sub-nano cluster catalysts, which hold great promise as they are economical and can be highly active. I will show that, under the influence of catalytic temperatures, pressures, presence of solvent or electrolyte, and/or electrochemical potential, such catalysts populate many distinct structural and stoichiometric states, which form a statistical ensemble that evolves together with the catalysed reaction. Metastable states in this ensemble play a key role in catalysis, and dictate the catalytic activity, selectivity, and durability, while the most stable form (the usual focus of research) can be catalytically irrelevant. Many rules of catalysis need a revision within this new paradigm. Scaling relations routinely break down, and that actually can be used strategically in catalyst design. Phase diagrams contain many structures per phase. *Operando* spectra need to be interpreted differently. The theory of Ostwald ripening needs to be extended. Most importantly, the catalytic mechanism is not one, but a swarm of many.

Several catalytic systems will be used to illustrate these points: semiconductor-supported Pt clusters and cluster alloys used for hydrocarbon dehydrogenation for endothermic cooling in aviation, and clusters of Pt, Pd, Au, Ag supported on graphite used for ORR catalysis. The talk will contain a mix of theory and experiment.

**Bio:** Anastassia Alexandrova is a Professor and Vice Chair in the Department of Chemistry and Biochemistry, UCLA.

She obtained a B.S./M.S. Diploma with highest honors, from Saratov University, Russia, her Ph.D. in theoretical physical chemistry from Utah State University, and was then a Postdoctoral Associate and an American Cancer Society Postdoctoral Fellow at Yale University.

Anastassia joined the faculty of UCLA and CNSI in 2010. The focus of her laboratory is theory and computation for design and multi-scale modeling of functional materials: dynamic catalytic interfaces, artificial metalloenzymes, molecular qubits and their assemblies, and quantum materials. She is a recipient of numerous awards, such as NSF CAREER Award, Sloan Fellowship 2013, DARPA Young Faculty Award 2011, Fulbright Fellowship 2016, and ACS WCC Rising Star Award 2016, 2020 ACS Phys Early Career Award in Theoretical Chemistry, 2021 Max Planck-Humboldt medal, as well as UCLA's Hanson-Dow award for excellence in teaching 2016, Herbert Newby McCoy award for excellence in faculty research 2016, undergraduate research mentorship award 2018, and 2019 distinguished teaching award (the highest honor for