



UNIVERSITY OF DELAWARE
ENGINEERING

DEPARTMENT OF CHEMICAL & BIOMOLECULAR ENGINEERING

CENTER FOR CATALYTIC SCIENCE AND TECHNOLOGY

www.che.udel.edu/ccst

SPRING WEBINAR



RACHEL GETMAN

CLEMSON UNIVERSITY
Murdich Family Endowed
Associate Professor of Chemical &
Biomolecular Engineering

**WEDNESDAY, MAY 5, 2021
at 10:00 AM (E.S.T)**

MOLECULAR-LEVEL INSIGHTS INTO HOW LIQUID WATER INFLUENCES CATALYTIC PHENOMENA AT WATER/ CATALYST AND WATER/ELECTROCATALYST INTERFACES

Multiple societally important chemical reactions rely on catalytic processing in aqueous conditions, including biomass processing, electrochemical energy conversion, fertilizer production, and water purification. A goal of our work is to learn the molecular-level ways in which solvent molecules influence catalysis, both so that we can better understand catalyst fundamentals and so that we can garner insight needed to design new catalysts and optimize catalytic operating conditions. Experiments and simulations have uncovered a variety of ways in which water solvent influences catalytic phenomena. For example, it alters reaction intermediate and transition state energies, co-catalyzes certain reaction steps, and controls which catalytic pathways are followed. However, a comprehensive picture about how H₂O molecules influence catalytic behavior, including their influence on catalytic energetics, remains unresolved. In this work, we use multiscale modeling involving density functional theory (DFT) and force-field molecular dynamics (ffMD) to examine how interfacial water influences the free energies of hydrophilic and hydrophobic adsorbates on hydrophobic Pt slabs, Pt electrodes, and supported Pt surfaces. We demonstrate how the polarities of the solvent, catalytic species, and catalyst interface influence catalytic enthalpies and entropies of solvation. Further, we show how solvents can be designed to control solvation thermodynamics in order to harness control over catalytic chemistry.

REGISTER HERE

NOTE: SEMINARS/WEBINARS ARE SCHEDULED AT EASTERN STANDARD TIMES (E.S.T.)