

The Department of Chemical Engineering Presents:



Understanding and Design of Solvation for Chemical Processes

Qing Shao

University of Kentucky

Wednesday, April 21, 2020

3:30PM via Zoom

<https://rochester.zoom.us/j/92532222592?pwd=OUdlOTczUzJjVUM5ZTFjcTRCTk9hUT09>

Abstract: This seminar will present computational research about the solvation effect. Many chemical and biological processes occur in a solvent or media (water, organic solution, or polymer matrix), such as substrate-enzyme interactions, nanomaterials aggregation, and polymer processing. The solvent molecules present non-bulk features around materials and exert a solvation effect that could determine the fate of the processes. Understanding the solvation effect and designing solvents with the desired effect is critical for developing the related processes from enzymatic reactions to polymer decomposition. This seminar will present two examples about the solvation effect using computation. The first example will present the research that aims to investigate the fundamental relationship between ionic solvation and hopping in polymer electrolytes. We will show the heterogeneity of ionic solvation and how the solvation of ions determines their conductivity. The second example will present the research that aims to understand the multiscale solvation effect of deep eutectic solvents in biomass decomposition. We will show the relationship between solvation and reactivity of lignin models. In addition, we will also present the development of a simulation-deep learning-experiment framework that can accelerate the discovery of new sustainable solvents.

Bio: Dr. Qing Shao obtained his Ph.D. with Dr. Shaoyi Jiang in Chemical Engineering at the University of Washington in 2014, then did postdoctoral research with Dr. Carol Hall at North Carolina State University. He started as an assistant professor in the chemical and materials engineering department at the University of Kentucky in 2018. His current research focuses on understanding and designing solvents for energy, environmental and biological applications using computational approaches. He was listed as the Emerging Investigator 2020 by the Journal of Materials Chemistry B of the Royal Society of Chemistry. Dr. Shao has authored or co-authored more than 40 papers (cited > 2000)