School of Molecular Sciences
Arizona State University

# SMS Fall 2021 Seminar Series

## Friday Oct 22 | 2:30pm | Biodesign Auditorium*

### Exploring Biological Mechanisms and Materials Through Molecular Simulation for a Sustainable Bioeconomy

Economic growth has for centuries been coupled to carbon emissions, timeshifting photosynthesis-driven biosynthesis from prehistoric times to today for fuel and materials. In order to mitigate the climatological impacts that increased carbon emissions have, it is imperative that we develop sustainable alternatives for current industrial processes. Leveraging plant biomass as an alternative raw material for commodity chemicals is an attractive alternative, with a potentially closed carbon cycle. However, our limited understanding of plant biomass at the molecular scale limits its utilization in practice. Through molecular simulation, we probe nanoscale interactions that stand in the way of utilizing biomass to its full potential. We focus primarily on the aromatic heteropolymer lignin found in plant cell walls and its interactions with other biopolymers. We quantify lignin interactions with cellulose, and explore organic solvent treatments to disrupt lignin-cellulose association. Molecular simulation also provides unique insight into the permeation of lignin small molecules through lipid bilayers, with implications for designing microbial lignin “biorefineries”. Avoiding lignin is also one of the key obstacles cellulose-degrading enzymes face. Together with experimental collaborators, we determined the unbinding mechanism for cellulases once bound to cellulose to allow these critical processive enzymes to avoid a lignin blockage, providing yet another example where computational insights are critical to testing mechanistic hypotheses.

## Josh Vermaas, PhD

***Assistant Professor, Michigan State University***

Josh Vermaas is a molecular scientist studying biological systems through molecular simulation. He graduated from Arizona State with a bachelors degree in Biochemistry, Physics, and Computational Math, and subsequently went to the University of Illinois to pursue a PhD in biophysics. While there, he had the opportunity through fellowships to work with scientists at the National Renewable Energy Laboratory, Oak Ridge National Laboratory, and Sandia National Laboratory. Following a Director’s Fellowship postdoctoral stint at the National Renewable Energy Laboratory, he was a computational scientist at Oak Ridge, working during 2020 to develop frameworks for gigadocking against SARS-COV-2 targets. Josh started his own independent laboratory at Michigan State University within the Plant Research Lab earlier this year, focusing on applying computational science broadly to plant research and sustainability efforts.

**ZOOM option available: https://asu.zoom.us/j/87081218152*