Rensselaer

The HOWARD P. ISERMANN
DEPARTMENT OF CHEMICAL AND
BIOLOGICAL ENGINEERING

CBE Seminar Series – Spring 2023

Dr. Tucker Burgin

Postdoctoral Fellow
University of Washington

Seminar: Wednesday, March 8, 2023
9:30 a.m. (Ricketts 203)

"*In silico* Enzyme Engineering: Molecular Simulation and Machine Learning for Rapid Screening and Discovery"

Abstract:

Enzymes are among the most promising tools available to address ongoing and emerging needs for sustainable, efficient, and cheap catalysis, and will play a central role in the forthcoming bioeconomy. However, enzymes are highly intricate macromolecules whose catalytic properties are often difficult to predict and engineer. Atomistic simulations of enzymes are an important tool for revealing the complex mechanisms underlying enzyme function, but they remain underutilized in screening for improved engineered variants due to a host of technical hurdles. In this talk I will describe contributions to the use of atomistic simulations for the discovery and characterization of unknown enzyme reaction mechanisms, and I will show how this knowledge can be extended through the use of creative simulations to greatly simplify the task of computationally screening the effects of enzyme mutations. I will then demonstrate how machine learning approaches to enzyme engineering can benefit from simulation data, both to directly speed up the search for promising enzyme variants and to complement other sources of information about enzymes, such as experiments and proteomics. Taken as a whole, this work lays the foundation for a new subdiscipline of computational enzyme engineering that synergizes with existing and emerging approaches to this important problem.

Biography:

Tucker Burgin is a Postdoctoral Fellow at the University of Washington, working with Professors Jim Pfaendtner and David Beck. He obtained his Ph.D. in Chemical Engineering in 2021 from the University of Michigan, where his research focused on the application of molecular simulations and scientific software engineering to uncovering enzyme mechanisms. He was supported during his graduate studies by two fellowships from the Molecular Sciences Software Institute (MolSSI), and he is currently a Data Science Fellow with the University of Washington eScience Institute. His research is exploring new opportunities at the intersection of molecular simulation, machine learning, and enzyme engineering.

Refreshments will be available at 9:00 a.m. in the Ricketts Coonley Lounge (RI 120).
For more information, please contact Lisa Martin (swishl@rpi.edu)