The Department of Chemical Engineering
Presents:

Professor Andrew White
Assistant Professor of Chemical Engineering
University of Rochester

Computational design of peptide-based materials with maximum entropy molecular simulation and data-driven modeling

ABSTRACT: Peptides are small proteins built from monomer units called amino acids. Peptides can be precisely synthesized using solid-phase peptide synthesis and their constituent amino acids can provide functional groups ranging from hydrogen bond-donors to aromatics. Peptides can be immobilized onto surfaces, nanoparticles, or formed into hydrogels. This flexibility and precise control give a wide-range of potential applications including self-assembling antifouling surface coatings, antimicrobial therapeutics, hydrogel vaccines, and nucleating crystal structures. In this talk, I will present computational methods my group has used to design peptides for antifouling, antimicrobial, and self-assembly. Our approach is to use insight from nature through data-driven informatics methods and maximum entropy molecular simulation. Molecular simulation seeks to model the dynamics of peptides at the atomic level. Maximum entropy methods minimally modify molecular simulations to match experimental data. This enables better accuracy, which is critical for modeling self-assembly of peptides, which is a complex multiscale process. Broadly our goal in methods development is to combine physics-based simulation with modern machine learning methods to create interpretable and accurate models. Most of our tools and methods are freely available and this talk will describe how they can be used for systems beyond peptides.

BIO: Dr. White graduated from Rose-Hulman Institute of Technology in 2008 with a BS in chemical engineering. While at Rose, he spent a year studying at the Otto-von Guericke Universität in Magdeburg, Germany. While there, he worked for six months in a microbiology lab at the Max Planck Institute for Dynamics of Complex Technical Systems with Professor Hartmut Grammel in Germany. Dr. White completed a PhD in chemical engineering at the University of Washington in 2013. The thesis topic was the creation of non-fouling surfaces with computational modeling. Next, Dr. White worked with Professor Greg Voth at University of Chicago as a Post-doctoral fellow in the Institute for Biophysical Dynamics from 2013-2014. In Chicago, he developed new methods for mixing simulations and experiments. Dr. White is currently and has been an assistant professor at University of Rochester since 2015. Dr. White enjoys jogging, snowboarding and sometimes graphical design. His artwork appeared in at the Visualization Center Museum in Sweden in 2013.

Wednesday, January 30, 2019, 3:25 PM
Gavett Hall Room 202