DEPARTMENT OF CHEMISTRY AND ENVIRONMENTAL SCIENCE
SEMINAR SERIES
SPRING 2019

DATE: THURSDAY, FEBRUARY 21
LOCATION: WEC Lecture Hall
TIME: 3:00pm – 4:00pm

GUEST SPEAKER

Dr. Jodi Ann Hadden
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TOPIC

Elucidating the mechanisms of molecular machines through the computational microscope

ABSTRACT

At the technological interface of chemistry, physics, biology, and computing, there exists the only scientific instrument capable of characterizing the dynamical properties of biomolecular systems at atomic resolution. The computational microscope, realized through the application of supercomputers to perform all-atom molecular dynamics simulations, has emerged as a powerful tool to investigate the complex cellular machinery that supports life, as well as the pathogenic systems that threaten it. In this body of work, the computational microscope is leveraged to reveal key insights -- inaccessible to experimental methods -- into host-cell adhesion by the influenza virus hemagglutinin, the mechanism of intracellular cargo trafficking by cytoplasmic dynein, and the functional dynamics and drug-induced disruption of the hepatitis B virus capsid. Using simulations, we have discovered a role for extended glycan-receptor structure in hemagglutinin host recognition, the mechanical interplay of the dynein linker and stalk domains that drives directed cargo transport, and chemical-physical properties of the hepatitis B virus capsid that support its ability to accommodate genome maturation and control the display of cellular signals. By allowing researchers to elucidate the atomistic mechanisms of molecular machines of fundamental importance to human health, the computational microscope will increasingly enable the realization of novel strategies to address disease and the rational design of new treatments.

BIO

Following her undergraduate training in Chemistry (BS, 2007), Jodi completed her doctoral work in Computational Chemistry with Robert Woods at the University of Georgia (PhD, 2014), where she specialized in modeling and molecular dynamics simulations of carbohydrates, glycoproteins, and protein-carbohydrate complexes. During her postdoctoral phase with Klaus Schulten at the University of Illinois at Urbana-Champaign, she broadened her expertise to include large-scale molecular dynamics simulations of biomedically-relevant proteins and multimeric protein complexes, focusing on the dynamical properties of molecular machines. Since August 2017, Jodi has been funded by a special postdoctoral fellowship from the University of Delaware that supports her to perform computational research of her own design, independent of an academic advisor. Her current research projects focus on the drug-induced disruption of the hepatitis B virus capsid and the mechanism of the cytoplasmic dynein motor.

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