

DEPARTMENT OF CHEMISTRY AND ENVIRONMENTAL SCIENCE
SEMINAR SERIES
SPRING 2019

DATE: THURSDAY, FEBRUARY 14

LOCATION: WEC Lecture Hall

TIME: 3:00pm – 5:00pm

GUEST SPEAKER

Dr. James McCarty

Postdoctoral Fellow/Shea Group

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Santa Barbara, CA

TOPIC

Fluctuations, Rare Events, and Supramolecular Assemblies: Computational Approaches for Biomolecular and Materials Simulation

ABSTRACT

A fundamental goal of physical science is to understand how molecular chemistry gives rise to the large-scale structural and dynamic properties of complex condensed-phase systems. Such systems are often characterized by transiently populated metastable states that are difficult to sample using conventional molecular dynamics. In this seminar, I will survey strategies based on statistical mechanics that I have developed, with the goal of extending the capability of computer simulation for studying long-time behavior at macromolecular to sub-cellular levels. The inherent high dimensionality of biomolecules makes them challenging for sampling methods, such as metadynamics, that rely on a reduced set of collective variables. I will present an approach to obtain efficient collective variables that can illuminate the underlying physics of such systems. Then, I will describe how to obtain kinetic properties of infrequent events using a powerful variational formalism. Finally, moving to the mesoscopic regime, I will discuss a polymer field theoretic approach to study biomolecular aggregates of intrinsically disordered proteins. This work opens up the realm of simulations to study liquid-liquid phase separation in biology.

BIO

James McCarty received his Bachelor of Science with honors from the California Polytechnic State University in San Luis Obispo, CA and his Ph.D. in Chemistry from the University of Oregon where he did his doctoral work in theoretical physical chemistry under the supervision of Prof. Marina Guenza. After completing his Ph.D., he joined the group of Prof. Michele Parrinello as a postdoctoral associate in the Department of Chemistry and Applied Biosciences at ETH Zürich, Switzerland. He currently holds a postdoctoral fellowship at the University of California, Santa Barbara, in the group of Prof. Joan-Emma Shea, where he has a joint appointment in the Department of Chemistry and Biochemistry, the Materials Research Laboratory, and the Neuroscience Research Institute at UCSB. His research interests include molecular dynamics simulation, enhanced sampling of rare events, and polymer physics.

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