

Amgen Seminar Series in Chemical Engineering
in
Cherry Auditorium, Kirk Hall, 12:45 PM

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**Recent simulation methods for resolving molecular details
in thermodynamics and kinetics**

By



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Molecular dynamics (MD) simulations are increasingly powerful tools for augmented thinking about molecular-level phenomena and their links to macroscopic properties. Fundamentally, MD propagates atomic positions and velocities by numerical integration of equations of motion subject to forces representing interatomic interactions. Unfortunately, even with present day computational power, it is nearly impossible to directly observe phenomena that have natural timescales of greater than about a microsecond or length scales greater than a few tens of nanometers using MD. This is because the ceaseless thermal agitation resolved by MD only very rarely and unpredictably rectifies itself along productive directions in some more macroscopically meaningful variable space. Our group is devoted to overcoming this issue with novel methods that provide access to these “rare events” with the ultimate aim being a full description of the equilibrium distributions and transition rates in some state space of interest. In this talk, I will highlight the development and application of some of these modern MD techniques, including temperature-acceleration and Markovian milestoneing. Applications to be touched on include ligand entry and exit kinetics in enzymes and transmembrane ion transport. I will close with some highlights of future directions in method developments that involve hybrid approaches.

SPEAKER BIO: Cameron F. Abrams is a Professor and the Department Head of Chemical and Biological Engineering at Drexel University in Philadelphia. He received a BS in Chemical Engineering from North Carolina State University in 1995 and a PhD in Chemical Engineering from the University of California—Berkeley in 2000. After two years of postdoctoral training at the Max-Planck-Institute for Polymer Research in Mainz, Germany, he joined the Department of Chemical and Biological Engineering at Drexel University in Philadelphia as an Assistant Professor in 2002. Abrams’ primary research expertise lies in molecular simulations and new simulation method development, with applications ranging from new materials and fluids to drug design. Abrams is the recipient of an ONR Young Investigator Award, an NSF CAREER Award, and was the 2015 Impact Award Winner in the Computational Molecular Sciences and Engineering Forum of the American Institute of Chemical Engineers. In addition to novel molecular simulation methods, Abrams’ research interests include high-performance materials, protein-related kinetics and thermodynamics, and HIV-1 entry inhibitor design.

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