“Data-driven Design of Self-assembling Colloids and Machine Learning of Protein Folding Funnels”

Wednesday
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3:00 pm
Wu and Chen Auditorium
Levine Hall

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Abstract

The Data-driven modeling and machine learning have opened new paradigms and opportunities in the understanding and design of soft and biological materials. Colloidal particles with tunable anisotropic surface interactions are of technological interest in fabricating responsive actuators, biomimetic encapsulants, and photonic crystals with omnidirectional band gaps. In the first part of this talk, I will describe our applications of nonlinear manifold learning to determine low-dimensional assembly landscapes for self-assembling patchy colloids. These landscapes connect colloid architecture and prevailing conditions with emergent assembly behavior, and enable inverse building block design by rational sculpting of the landscape to engineer the stability and accessibility of desired aggregates. Rational engineering of structural and functional polymers and proteins requires an understanding of the underlying free energy landscapes dictating thermodynamic stability and kinetic folding pathways. In the second part of this talk, I will describe an approach integrating ideas from dynamical systems theory and nonlinear manifold learning to reconstruct multidimensional protein folding funnels from the time evolution of single experimentally-measurable observables.

Bio

Andrew Ferguson is an Associate Professor at the Institute for Molecular Engineering at the University of Chicago. He received an M.Eng. in Chemical Engineering from Imperial College London in 2005, and a Ph.D. in Chemical and Biological Engineering from Princeton University in 2010. From 2010 to 2012 he was a Postdoctoral Fellow of the Ragon Institute of MGH, MIT, and Harvard in the Department of Chemical Engineering at MIT. He commenced his independent career in the department of Materials Science and Engineering at the University of Illinois at Urbana-Champaign in August 2012, and was promoted to Associate Professor of Materials Science and Engineering and Chemical and Biomolecular Engineering in January 2018. He joined the Institute for Molecular Engineering in July 2018. His research uses theory, simulation, and machine learning to understand and design self-assembling materials, macromolecular folding, and antiviral therapies. He is the recipient of a 2017 UIUC College of Engineering Dean's Award for Excellence in Research, 2016 AIChE CoMSEF Young Investigator Award for Modeling & Simulation, 2015 ACS OpenEye Outstanding Junior Faculty Award, 2014 NSF CAREER Award, 2014 ACS PRF Doctoral New Investigator, and was named the Institution of Chemical Engineers North America 2013 Young Chemical Engineer of the Year

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