Seminar Announcement

Machine Learning Collective Variable Discovery for Materials Design and Engineering

Professor Andrew Ferguson
Molecular Engineering
University of Chicago

Time: 4:00—5:00 pm
Date: Wednesday, September 5, 2018
Venue: 136 DeBartolo Hall

Abstract

Data-driven modeling and machine learning have opened new paradigms and opportunities in the understanding and design of soft and biological materials. The automated discovery of emergent collective variables within high-dimensional computational and experimental data sets provides a means to understand and predict materials behavior and engineer properties and function. In the first part of this talk, I will discuss our use of auto-encoding deep networks to perform on-the-fly collective variable discovery and accelerated sampling of free energy landscapes in molecular dynamics simulation of proteins. In the second part of this talk, I will describe our use of nonlinear manifold learning to determine low-dimensional assembly landscapes for self-assembling patchy colloids and rationally sculpt these landscapes to engineer the stability and accessibility of desired polyhedral aggregates and open colloidal crystals with omnidirectional band gaps.

Biography

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.