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BIOENGINEERING

PRESENTS

Machine learning in soft and biological materials: Engineering self-assembling colloids and viral phase behavior

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2101 ENGINEERING V

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ABSTRACT:

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 soft responsive actuators, biomimetic polyhedral encapsulants, and substrates for high-density information storage. In the first part of this talk, I will describe our applications of nonlinear manifold learning to determine low-dimensional "assembly landscapes" from computer simulations and experimental particle tracking data for self-assembling patchy colloids. These landscapes connect colloid architecture and prevailing conditions with emergent assembly behavior, informing how to engineer the stability and accessibility of desired aggregates. Empirical models of viral fitness present a means to rationally design antiviral therapeutics by revealing vulnerabilities within the viral proteome. In the second part of this talk, I will discuss the translation of clinical sequence databases into spin glass models of viral fitness that reveal an interesting connection with statistical thermodynamics in which a data-driven fitness model of HIV admits an "error catastrophe" – mutational meltdown of the viral quasispecies induced by an elevated mutation rate – isomorphic to a first order phase transition. Our work informs new antiviral control strategies and provides a rationale for why HIV can live on the precipice of the error catastrophe with impunity.

BIOGRAPHY:

Andrew Ferguson is Assistant Professor of Materials Science and Engineering, and an Affiliated Assistant Professor of Chemical and Biomolecular Engineering, and Computational Science and Engineering at the University of Illinois at Urbana-Champaign. 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 appointment at UIUC in August 2012. His research interests lie at the intersection of materials science, molecular simulation, and machine learning, with particular foci in the design of antiviral vaccines and self-assembling colloids and peptides. 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.