



Seminar/Talk

Learning Thermodynamics from Sequence: Predicting and Designing Complex Biomolecular Mixtures

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Host: Carl Goodrich

Biological and bio-inspired materials derive function from sequence-encoded interactions in multicomponent mixtures. Predicting how biomolecular sequences determine thermodynamic behavior and material properties is therefore a central challenge across biophysics and molecular engineering. In this talk, I introduce a machine-learning framework that maps sequences directly to context-dependent chemical potentials—without requiring direct free-energy calculations. The approach learns low-dimensional, physically interpretable representations in which distances encode differences in thermodynamic behavior across mixtures. Using intrinsically disordered proteins as a model system, I demonstrate how this framework enables quantitative prediction of partitioning and multicomponent phase diagrams, while revealing how sequence composition and patterning jointly control mixture thermodynamics. More broadly, this work outlines a path toward quantitative models of complex mixtures that bridge machine learning, biophysics, and molecular engineering.

Thursday, October 22, 2026 11:00am - 12:00pm

ISTA | Central Building | Ballroom



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