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## An Information-driven Approach to Quantifying and Controlling Emergent Order

**Monday July 18th**
Lecture 4:00-5:00 p.m. | Physics/Astronomy Auditorium (PAA) A118
Reception 5:00-6:00 p.m. | Benson Hall Lobby

## Bio

Ashley Guo is a Postdoctoral Associate in the Center for Soft Matter Research at New York University, where she works in the lab of Professor Paul Chaikin. Her current research focuses on studying the dynamical absorbing state model known as Biased Random Organization and characterizing the phase transitions and ordering that emerge in this model using an information theoretic approach. Ashley obtained her Ph.D. from the Pritzker School of Molecular Engineering at the University of Chicago, where she worked with Professor Juan de Pablo. Her Ph.D. research focused on molecular simulations of protein aggregation and the development of enhanced sampling methods aided by machine learning approaches. Prior to her Ph.D., she completed her B.S. in Chemical Engineering at Caltech.

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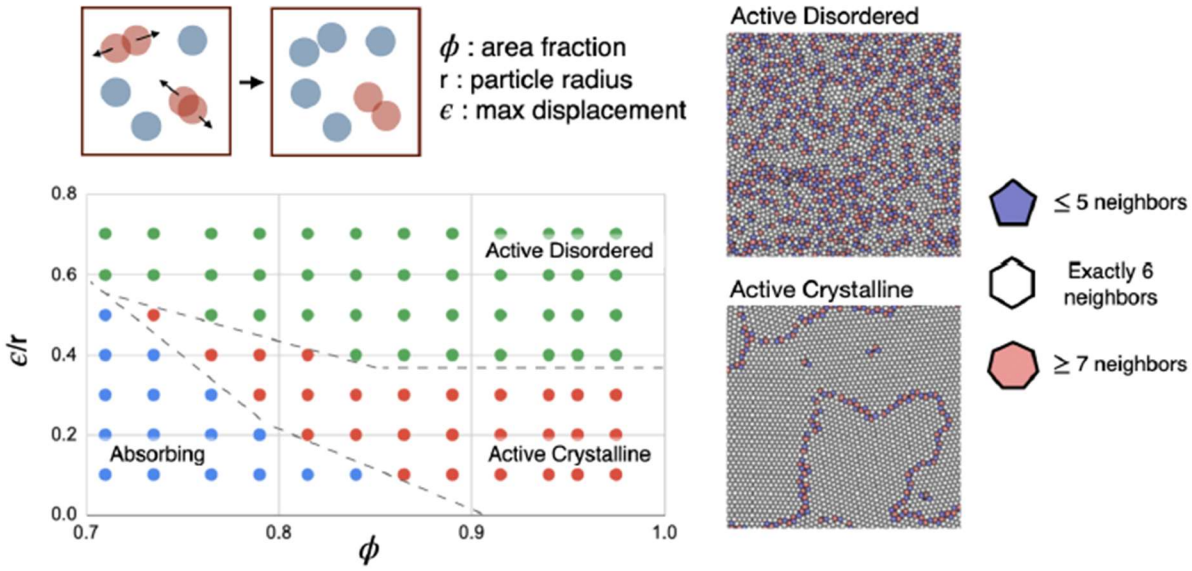
## Abstract

Controlling the emergence of order out of disorder is an overarching goal in the engineering of biological and soft materials. Examples in which such control has been targeted include the design of self-assembling functional materials such as metal organic frameworks [1], as well as the identification of strategies to halt aggregation of disease-implicated unstructured proteins [2]. Computational approaches traditionally rely on simulations at varying time and length scales, aided by enhanced sampling techniques [3], including the recent proliferation of machine learning based methods [4-6]. An exciting direction in the computational design of soft materials incorporates ideas from information theory into these approaches, drawing upon the connection between thermodynamic entropy and information entropy. In this talk, I consider a simple case with an information-driven analysis, which may inform future studies of real systems with greater complexity.

Here, I will discuss the emergence of order in a continuous dynamical absorbing state model known as Biased Random Organization (BRO), in which overlapping particles are considered active and are repelled apart by a random distance. This results in a phase transition between absorbing states containing no active particles and active states where particles continue to be displaced. I will focus on the behavior of BRO in 2D, which results in two distinct active phases unlike in other dimensions [7]. One such active phase is crystalline, which emerges when particles are repelled from their overlapping neighbors by small random magnitudes. The second active phase is disordered, which results from repulsive displacements with large random magnitudes. Although this phase is disordered, I will show that unlike in the crystalline phase, it exhibits hyperuniformity at criticality, a form of "hidden order" characterized by vanishing density fluctuations that holds potential for unique optical properties. As part of characterizing the three phase transitions found in 2D BRO, I apply a computable information density approach, in which a data compression algorithm is used to quantify changes in the system entropy. I will conclude with my plan for extending this approach to the computational study and design of self-assembling materials.

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