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Nonlinear machine learning in soft materials engineering and design[1]

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The inherently many-body nature of molecular folding and colloidal self-assembly makes it challenging to identify the underlying collective mechanisms and pathways governing system behavior, and has hindered rational design of soft materials with desired structure and function. Fundamentally, there exists a predictive gulf between the architecture and chemistry of individual molecules or colloids and the collective many-body thermodynamics and kinetics. Integrating machine learning techniques with statistical thermodynamics provides a means to bridge this divide and identify emergent folding pathways and self-assembly mechanisms from computer simulations or experimental particle tracking data. We will survey a few of our applications of this framework that illustrate the value of nonlinear machine learning in understanding and engineering soft materials: the non-equilibrium self-assembly of Janus colloids into pinwheels, clusters, and archipelagos; engineering reconfigurable "digital colloids" as a novel high-density information storage substrate; probing hierarchically self-assembling -conjugated asphaltenes in crude oil; and determining macromolecular folding funnels from measurements of single experimental observables. We close with an outlook on the future of machine learning in soft materials engineering, and share some personal perspectives on working at this disciplinary intersection.

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