Understanding diffusion processes in soft materials using machine learning

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Diffusion processes play a key role in the self-assembly and function of soft materials. It is known that diffusion processes are strongly dependent on the underlying mesoscale structure of such materials; however, understanding this dependence can be challenging when the structure itself is difficult to characterize. Machine learning can help uncover and interpret the tightly coupled relationships between complex structures and processes. Here, I will discuss the use of an unsupervised characterization approach to identify assembly mechanisms in colloidal crystals produced by drying (an advection–diffusion process). I will then discuss the use of regression to identify morphological features of triblock copolymer water-treatment membranes that control solute self-diffusion. In both cases, machine learning helps understand diffusion processes that would be otherwise challenging to analyze.