Self-assembly and emergent phenomena using nanoparticles and anisotropic colloids

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Materials science exploits self-assembly to achieve novel physical properties. Progress in chemical synthesis and characterization has rapidly increased the control over how matter organizes on the nanoscale. In this talk I present computational work on the self-assembly of nanoparticles and colloids. A particular focus is the role of particle shape and entropically driven self-assembly. I will show results for idealized model systems (hard particles, pair potentials, in and out of equilibrium), as well as discuss work on modeling conducted in collaboration with experimentalists. Our computational tools are molecular dynamics and Monte Carlo simulations on CPUs or accelerated with GPUs using in-house code. Visualization plays an important role to discover and characterize complex structures. If time permits, I will demonstrate interactive simulations and structure solution.

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