ENGINEERING ORDER THROUGH ENTROPY: ROLE OF PARTICLE SHAPE ANISOTROPY IN ASSEMBLY AND DYNAMICS

Purely entropic (excluded volume) interactions drive disorder-order transitions in certain colloidal assemblies. Numerous studies on self-assembly of natural and man-made supramolecules underline the fact: highly ordered and complex structures have arisen in nature not despite of entropy but because of it._ Understanding and controlling these weak yet 'boundless' interactions in addition to the strong but 'finite' enthalpic interactions is the key to devise strategies for fabrication of numerous hierarchical-functional materials such as nanocrystal solar cells, mesoporous catalysts, membranes, smart materials, high performance plastics etc. While order-disorder transitions are controlled by a delicate balance of enthalpic and entropic changes, for hard particles there are no enthalpic forces hence excluded volume interactions due to shape anisotropy solely dictate their phase behaviour and dynamics.

To understand the basic principles controlling formation of these hard particle assemblies, we performed systematic simulation studies to explore the effect of ’shape’ or excluded volume interactions on the equilibrium mesophase behavior and on selected non-equilibrium mechanical properties of these systems. Guidelines for predicting phase behavior based on certain geometrical attributes of shapes, effect of size and shape polydispersity on order-disorder transitions and effect of anisotropy on microstructural relaxation and certain macroscopic mechanical properties are established. Together, these findings make a stride towards general understanding and classification of the effect of particle shape on thermophysical properties of its assemblies.