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Self-assembly of confined nanoparticles in bipolar nematic liquid crystal droplets.

Abstract:

The balance between liquid crystal mediated forces and entropic frustration is studied during the self-assembly of Nano-particles on the surface of bipolar nematic liquid crystal droplets. The free energy functional of the liquid crystal is described in the framework of the Landau-de Gennes formalism, where Monte Carlo and Ginzburg-Landau relaxation methods are used to explore local and global minima with their respective appearance probability. A novel Metropolis sampling algorithm is used to minimize the free energy functional by generating a Markov chain of states in function of the alignment tensor and the position of the particles. We explore systems where homeotropic and planar anchored Nano-particles are half-submerged in a degenerative planar liquid crystalline droplet. We observe that homeotropic particles are located at the droplet boojums to decrease the total free energy to an amount around a thousand k B T units. Similarly, weak planar anchored particles prefer the boojums, relaxing the free energy several hundreds of kBT units. Our results consolidate and explain previous experimental observations about the nematic induced assembly of particles in micron sized droplets and aid in the design of liquid crystal based technology for the direct assembly of structured materials.