Entropy stabilized quasicrystalline-like arrangements of spherical micelles

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Polymer-tethered nanoparticle "shape amphiphiles" provide a novel approach to control the self-assembly of nanoparticles into phases reminiscent of those seen in surfactants and block copolymers, such as ordered arrangements of spherical micelles. Here we present the results of Brownian dynamics simulations used to investigate nanospheres functionalized with a single tether, in a solvent poor for the tethers and good for the nanoparticles. We explore the region where mono-tethered nanospheres self-assemble into spherical micelles which in turn self-assemble into a dodecagonal quasicrystal approximant - a structure not previously reported for block copolymers and related amphiphiles. We propose a simple entropic model to explain this tendency towards quasicrystalline order, explore the behavior of this model system using simulation, and present a general mechanism for the formation of quasicrystals in soft matter systems.