Self-assembly of micro-capsules formed by nanoparticles via liquid crystal sorting

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We study nanoparticles dispersed in pentyl-cyano-biphenil (5CB). When nanoparticles are functionalized with calamitic mesogens, they disperse uniformly in the isotropic phase of 5CB but in the nematic phase they form a micron-sized shell enveloping nematic droplets, surrounded by a continuous nematic phase. In order to explain this assembly, we present thermodynamic models and Monte Carlo simulations, minimizing the free energy of the system in terms of the alignment of the liquid crystal inside the shell and the packing fraction of the nanoparticles in the shell. We show that formation of the micro-shells can be understood as a first-order structural transition where the latent heat of nematization competes with the excluded volume of the nanoparticles. For applications in controlled delivery, we provide insight for controlling the formation and characteristics of the micro-shell wall in terms of experimental quantities.