Self-assembly of colloidal dimers around spherical nanoparticles: a simple model for encapsulation

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In the last years, the mechanism of formation of a coating layer (nanocapsule) around a target species is capturing large fundamental and technological interest; to quote few applications, encapsulation is essential in the pharmaceutical field, where it plays an important role in drug delivery in the human body [1], or as a means to protect proteins, peptides and DNA from contact with the external environment [2]; in food industry, encapsulation may be used to preserve the quality of nutraceuticals [3]. One of the way to design encapsulating structures relies on their spontaneous appearance through self-assembly. In this context, the self-assembling properties of amphiphilic molecules, lipids, colloids and protein-like copolymers are very promising [4]. Here we present a Monte Carlo simulation study of the coating process of colloidal dimers onto spherical nanoparticles. To this end we investigate a simplified mixture of hard spheres (the guest particles) and hard dimers formed by two tangent spheres of different size (the encapsulating agents); in our scheme, the implicit role of the solvent is to provide an effective attraction between the smaller particle of a dimer and a guest sphere, whose range depends on their relative size. By tuning the size and concentration of guests, under overall dilute conditions a rich phase behavior emerges: for small sizes and/or low concentrations, the preferred arrangement is to form compact aggregates (capsules) of variable sizes, where one or few guest particles are coated with dimers; for larger sizes and moderate guest concentrations, other scenarios are realized, including equilibrium separation between a guest-rich and a guest-poor phase. Our results serve as a framework for a more systematic investigation of self-assembled structures of functionalized dimers capable of encapsulating target particles, like for instance noble proteins in a colloidal dispersion.

\textbf{Figure} Typical self-assembled capsules resulting from simulation upon increasing the guest size.