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

Gianmarco Munaò*, Dino Costa, Santi Prestipino, Carlo Caccamo

Dipartimento di Scienze Matematiche e Informatiche, Scienze Fisiche e Scienze della Terra

Università degli Studi di Messina, Viale F. Stagno d'Alcontres 31, 98166 Messina (Italy)

**gmunao@unime.it*

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.

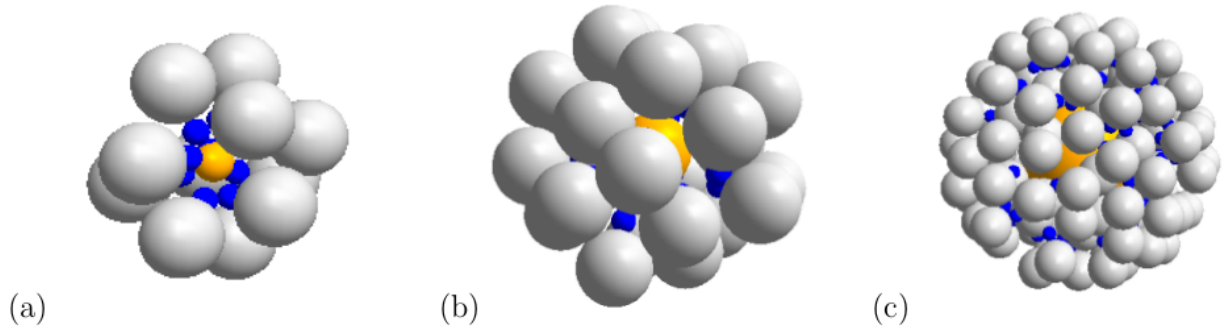

Figure 1 Typical self-assembled capsules resulting from simulation upon increasing the guest size.

[1] L. Zhang et al., *ACS Nano,* 2008, **2**, 1696.

[2] S. D. Perrault and W. M. Shih, *ACS Nano,* 2014, **8**, 5132.

[3] M. A. Augustin and Y. Hemar,*Chem. Soc. Rev*., 2008, **38**, 902.

[4] R. Malik, J. Genzer and C. K. Hall, *Langmuir,* 2015, **31**, 3518.