Journal of
Thermodynamics & Catalysis
ISSN: 2157-7544

Editorial
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Self-assemby of Janus Particles

J. D. Gunton*

Department of Physics, Lehigh University, USA

One of the exciting developments in several fields of science these days is the design of so-called smart materials, whereby particles are initially coded in such a way as to guide the self-assembly process. By this method one can design and control the desired properties of a substance. In this article I briefly review one such method of encoding, based on an original idea of the brilliant French theoretical physicist, P.G.de Gennes. In his 1992 Nobel acceptance speech, he pointed to the exciting potential, for both science and technology, of Janus spheres whose chemical makeup differs between the two hemispheres. These particles were named after the Roman god who has two faces looking into opposite directions, to describe a special class of colloidal particles with different chemical make ups on their two hemispheres. De Gennes imagined that these amphiphilic Janus particles might behave like surfactant molecules to adsorb at the water air interface, forming a monolayer that de Gennes described as a skin that can breathe, since small molecules would still be able to diffuse through the interstices between the Janus particles in the monolayer. These ideas were largely ignored in subsequent years due to the lack of proper synthetic methods to fabricate Janus particles. However, eventually scientists have found clever ways to synthesize Janus spheres and the field has subsequently seen significant developments. A paper by Granick and collaborators in Advanced Materials in 2010 discusses recent progress regarding the synthesis and self-assembly of Janus particles, including theoretical and simulation studies.

The general field of designing smart materials has been receiving considerable attention recently. Various site-specific techniques such as template-assisted fabrication and physical vapor deposition have been developed to synthesize patchy colloidal particles of different shapes, patterns and functionalities. The self-assembly of those building blocks into a desired mesoscopic structure and function are considered as a bottom-up strategy to obtain new bulk materials that have potential applications in many fields including drug delivery, photonic crystals, biomaterials and electronics. The effects of anisotropy have been classified using the concept of an anisotropy dimension including patchiness, aspect ratio, faceting, etc. One particular example is the Janus sphere with two dissimilar semi-surfaces, which has been extensively studied experimentally and theoretically. Examples of dissimilar, coded surfaces include hydrophobic/hydrophilic, charged/uncharged, and metallic/polymer surfaces. A variety of stable structures and unusual phase behaviors have been found under different chemical conditions of the solution by both experiments and computer simulations. A primitive two-patch model has been used to model Janus spheres. In Monte Carlo simulations; this simplified model reproduces the main experimental features including self-assembly morphology and sheds light on potential applications in engineering and theoretical studies of reentrant phase diagrams.

Recent studies, including those of our group, explore the role of aspect ratio, in which patches are arranged on an anisotropic core such as spheroids. The anisotropy dimension is related to the aspect ratio and recent studies using ground-state energy calculations reveal many interesting structures, such as a helical shape. In experiments, ellipsoidal colloids can be engineered with high mono dispersity using techniques such as deforming the spherical silica by ion fluence, which makes the patched ellipsoidal surface possible if one can combine this with the template-assisted fabrication technique. Suspensions of ellipsoidal Janus particles provide a good candidate to study the effect of aspect ratio on self-assembly and new features of colloidal phase transformations.

As an illustration of some of these ideas, I will briefly discuss some recent simulation results of our group for ellipsoidal Janus particles. The lengths of the principle axes of the ellipsoids are denoted by a=b=c and the aspect ratio is defined as equal to a, To illustrate the dependence of aggregation morphology on the aspect ratio, we calculated the cluster distribution for several values of 0.1, 0.5, and 0.9, respectively. Our results show that for larger aspect ratio, the self-assembly process is relatively faster and the morphology is more

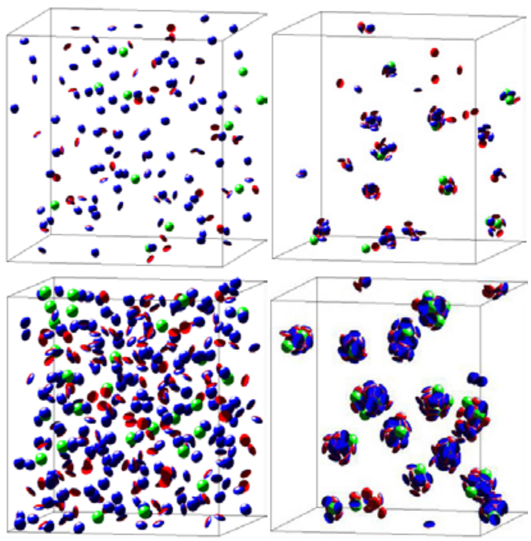

Figure 1: (color online). Morphology of entire system for ellipsoid aspect ratio=0.4. Red and blue colors denote hydrophobic and hydrophilic surfaces, respectively; green denotes the guest (drug) particle. (A) Initial configuration of number density ρ=0.01. (B) Encapsulation system (ρ=0.01) after 2.5 million MCS. (C) Initial configuration of number density ρ=0.06. (D) Encapsulation system (ρ=0.06) after 2.5 million MCS.

***Corresponding author:** J. D. Gunton, Department of Physics, Lehigh University, USA, E-mail: jdg4@Lehigh.EDU

Received May 03, 2012; **Accepted** May 08, 2012; **Published** May 08, 2012

Citation: Gunton JD (2012) Self-assembly of Janus Particles. J Thermodyn Catal 3:e106. doi:10.4172/2157-7544.1000e106

complicated, including chain structures, as well as micelles and vesicles that were found in earlier studies of spherical Janus particles. The structures for smaller aspect ratio are more uniform and multiple-layer vesicles dominate. We also find for small aspect ratio that ellipsoids tend to form vesicles, which suggest a potential application for particle encapsulation discussed below. Perhaps the most important result of the study for materials engineering is the fact that the size and structure of the aggregates can be controlled by the aspect ratio, which should be an interesting result from a design viewpoint.

There are several potential technological applications of self-assembling Janus particle systems, some of which are detailed in the progress report by Granick and collaborators mentioned earlier. These include the use of amphiphilic Janus particles as solid surfactants that adhere to the oil-water interface, thereby stabilizing emulsions and foams. Another potential application is to use modulated optical nano probes, whose optical properties are modulated by their rotational diffusion. These optical probes can obtain useful information about the local rheological properties of the environment. We conclude by illustrating one possible application, using work from our own group in which we examine the possibility of encapsulating drug particles by Janus particles. Since the hollow space at the center of ellipsoidal micelles is typically greater than for spherical micelles, we considered ellipsoidal Janus particles as the encapsulating agents and modeled the drug particles as spherical particles that interacted with both the ellipsoidal particles and themselves. Two typical runs for density $\rho=0.01$ and 0.06, with an ellipsoid aspect ratio=0.4, are presented in the Figure1.We found that ellipsoidal Janus particles provide a very efficient method to encapsulate these guest particles, with a maximum efficiency occurring at = 0.6. Although this field is still in its infancy, it does promise to be an active field of research for many years to come.