Phase diagrams of Janus particles with fixed orientations

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A Janus fluid generally refers to a system composed of particles divided into two hemispheres, each hemisphere-hemisphere interaction being described by a different potential. The study of this class of systems has become quite relevant due to its close relation with the hydrophobic-hydrophillic behavior shown by certain colloidal systems. A simple characterization of the general Janus model with the the potential being defined as attractive in one hemisphere and non-attractive in the other hemisphere may be used to study such systems. Additionally, if the orientation of the hemispheres is constrained to two possibilities (up or down), the system becomes a binary mixture of particles of species 1 (active hemisphere pointing up) and species 2 (active hemisphere pointing down). This is sketched in Fig. 1.

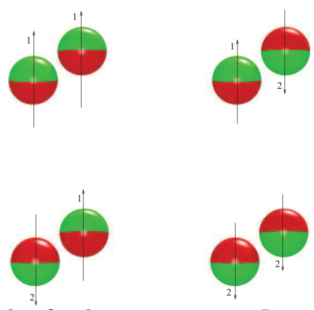

FIG. 1. Sketch of a binary-mixture Janus fluid with up–down constrained orientations.

We define the hemisphere-hemisphere interactions to be of square-well (SW) type. More explicitly, if a particle of species i is "below" a particle of species j (so that the top hemisphere of i interacts with the bottom hemisphere of j), the interaction potential is

$$\varphi_{ij}(r) = \begin{cases} \infty, & 0 \le r < \sigma, \\ -\epsilon_{ij}, & \sigma \le r < \sigma + \Delta, \\ 0, & \sigma + \Delta \le r, \end{cases} \tag{1}$$

where σ is the hard-sphere (HS) diameter, Δ is the width of the attractive well, and ϵ_{ij} is the depth of the well. By symmetry, one must have $\epsilon_{22} = \epsilon_{11}$ (see Fig. 1), so that (for given values of σ and Δ) the space parameter of the interaction potential becomes three-dimensional, as displayed in Fig. 2. We call $\epsilon = \max_{i,j}\{\epsilon_{ij}\}$ and use the three independent ratios ϵ_{ij}/ϵ as axes in Fig. 2. Next, without loss of generality, we choose $\epsilon_{12} \ge \epsilon_{21}$. With those criteria, all possible models of the class lie either inside the triangle SW-I0-B0-SW or inside the square SW-B0-A0-J0-SW.[1]

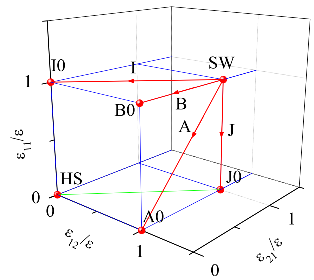

FIG. 2. Parameter space of the class of Janus models defined by Eq. (1).

This novel class of binary-mixture Janus fluids with up-down constrained orientations encompasses, as particular cases, the conventional one-component SW fluid, mixtures with isotropic attractive interactions only between like particles (model I0) or unlike particles (model J0), and genuine Janus fluids with anisotropic interactions and different patch-patch affinities (models A0 and B0).

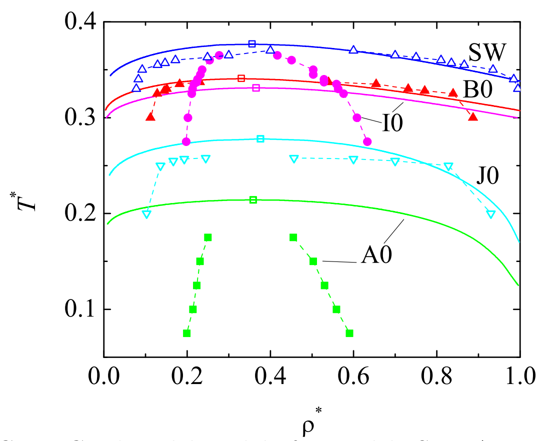

FIG. 3. Gas-liquid binodals for models SW, A0, B0, I0, and J0, as obtained from our theoretical method (solid lines) and from GEMC simulations (symbols).

In this work we focus on models SW, I0, J0, A0, and B0, and make and systematic study of the properties of the gas-liquid binodal (see Fig. 3) both from simple theoretical approaches[1,2] and from simulation results[1] obtained by means of the Gibbs ensemble Monte Carlo (GEMC) method.[3]

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