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Role of Laterally Shifted Dipoles in 3D Microstructure Formation of Janus Magnetic Colloids: Insights from Brownian Dynamics Simulations

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Self-assembly and dynamic reconfiguration are fundamental to designing nanostructured fluids with tunable microstructures. In this work, the three-dimensional microstructures of a dilute suspension of magnetic Janus colloids with a magnetic dipole laterally displaced from their center were studied using Brownian dynamics simulations. Microstructure and aggregation properties—including mean cluster size, nucleation and growth, cluster size distribution, orientational distribution, and effective cluster radius—were evaluated as a function of the dimensionless lateral dipolar shift (s). At small dipolar shifts ($s \rightarrow 0$), chain- and ring-shaped structures form, which are typically observed in particles with a centered dipole ($s = 0$). However, at intermediate dipolar shifts ($0.2 \leq s \leq 0.4$), the structures mainly form vesicles that, in some cases, coexist with rings and spherical micelles. Finally, for $s > 0.4$, spherical micelles are observed that progressively decrease in size as s increases, until small clusters of 2 or 3 particles are reached. For intermediate and high dipolar shifts, the typical power-law aggregation behavior breaks down, and the system saturates at small clusters. This study suggests that new microstructured fluids can be designed by controlling the dipolar displacement of their component colloidal particles, thereby influencing their microstructure and consequent macroscopic properties.

Primary author(s) : Dr DELACRUZ-ARAUJO, Ronal A. (Universidad Nacional Autónoma de Tayacaja Daniel Hernández Morillo)

Co-author(s) : Mr MENACHO-ABANTO, Jose F. (Universidad Nacional de Trujillo); Dr CÓRDOVA-FIGUEROA, Ubaldo M. (University of Puerto Rico - Mayagüez)

Presenter(s) : Dr DELACRUZ-ARAUJO, Ronal A. (Universidad Nacional Autónoma de Tayacaja Daniel Hernández Morillo)

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