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Hierarchical assemblies and cluster growth regimes of bipolar Janus nanoparticles: effect of particle characteristics
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Numerous current and potential applications have motivated fundamental understanding of self assembly of colloidal Janus particles (JP). Experimental studies on nano and micron sized JPs have demonstrated a plethora of simple and complex structures. However, computational approaches to date have lacked the sophistication required to capture the rich free energy landscape of suspension of JPs especially for nanoscale particles and hence have been unable to elucidate the underlying principles that govern their complex self assembly. In this study, molecular dynamic simulation of a restricted primitive model, which also includes long range columbic interaction, has been performed in order to elucidate the underlying physics in the self assembly of bipolar JP at different surface charge density (0.2∼1.3 e/nm2) , salt concentration(0∼3 mM) and particle sizes. Our results clearly indicate formation of two distinct sub structures in very low JP concentration, namely: strings and rings. As the concentration of JP increases these sub structures joins and/or hierarchically assemble into larger clusters. Furthermore, the interconnection between the ionic cloud around a single JP and sequential cluster growth in JPS as a function of surface charge density, particle size and steric hindrance of surface ions has been elucidated.

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