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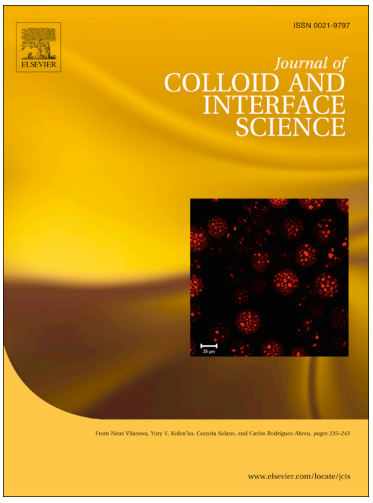

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Computer simulations of heteroaggregation with large size asymmetric colloids

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Abstract

Hypothesis:
Hetero-aggregation of inorganic colloids is influenced by numerous parameters, which dictate the suspension properties. When particles are different in size, the suspension can be either stable or unstable according to concentration of components, ionic strength, and pH. Experimentally, understanding the role of each parameter is sometimes difficult because parameters can not easily be modified independently. Numerical simulations are thus very useful to discriminate between different effects.

Simulations:
Brownian dynamics simulations are used here to study the heteroaggregation of dilute suspensions composed of two populations of colloids with large size asymmetry. Special attention is paid to the effect of small-particle concentration, surface potentials, and ionic strength.

Findings:
The simulation results show that hetero-aggregation can be tuned by modifying these different parameters, and that the resulting aggregate structures depend more on the surface properties of small particles than on those of large particles. The simulations shed light on a further parameter crucially influencing heteroaggregation, i.e. the mobility of small particles when adsorbed on large ones. The present results rationalize numerous experimental observations reported in the literature and can be used as reference to explain future experimental observations.

Keywords: Brownian Dynamics simulations, colloidal suspensions, heteroaggregation, aggregate structures, size-asymmetric particles

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