Coadsorption of Counterionic Colloids in Gibbs Monolayers: A Coarse-Grained Simulation Study.

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Monolayers of oppositely charged colloids form versatile self-organizing substrates, with a recognized potential to tailor functional interfaces. Here we present a coarse-grained Monte Carlo simulation approach to evaluate the thermodynamic and structural properties of Gibbs monolayers, in which one of the counterionic species is partially soluble [1,2]. With our methodology we have observed that the composition of this type of monolayer varies in a nontrivial way with surface coverage, as a result of a subtle competition between steric and attractive forces. In the regime of weak electrostatic interactions, the monolayer is depleted of soluble colloids as the surface coverage is increased. At sufficiently strong interactions, the incorporation of soluble colloids is favored at high surface coverage, leading to a re-entrant-type behavior in the expansion/compression isotherms. Strong electrostatic interactions also favor the clustering of the colloids, leading to a range of aggregated configurations, qualitatively resembling those obtained in previous experimental studies. At sufficiently high surface coverage, the clusters collapse into a gel-like percolated mesoscopic structure and eventually into a square crystal lattice configuration. Such interfacial structures are in good agreement with the ones observed in the few experimental investigations available for these systems, showing that the simple methodology introduced in this study provides a valuable predictive framework to anticipate the landscape of interfacial structures that may be produced with oppositely charged colloids, through the modulation of pair interactions and thermodynamical conditions.

Referencias

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