



Simple models of complex aggregation: vesicles formation by soft repulsive spheres with dipole-like interactions

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[摘要] Structural and thermodynamic properties of spherical particles carrying classical spins are investigated by Monte Carlo simulations. The potential energy is the sum of short range, purely repulsive pair contributions, and spin-spin interactions. These last are of the dipole-dipole form, with however a crucial change of sign. At low density and high temperature the system is a homogeneous fluid of weakly interacting particles and short range spin correlations. With decreasing temperature particles condense into an equilibrium population of free floating vesicles. The comparison with the electrostatic case, giving rise to predominantly 1D aggregates under similar conditions, is discussed. In both cases condensation is a continuous transformation, provided the isotropic part of the interatomic potential is purely repulsive. At low temperature the model allows to investigate thermal and mechanical properties of membranes. At intermediate temperatures it provides a simple model to investigate equilibrium polymerisation in a system giving rise to predominantly 2D aggregates.

[关键词] thermodynamic properties; simple model

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