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FLUCTUATION-DISSIPATION BROWNIAN DYNAMICS SIMULATION OF AGGLOMERATING ZINC OXIDE NANOPARTICLES IN WATER USED FOR THE CREATION OF NANOPHOTONICS MATERIALS

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The aim of this work was to develop a method for the theoretical description of many-particle interaction in nanocolloids, allowing to explore the formation of nano aggregates morphologies at the initial stage of nanoparticle coagulation.

An original phenomenological linear charge regulation model based on a preliminary experimental study of the modeled system was used in the presented study to describe the process of charge redistribution on the surfaces of interacting nanoparticles and in their electrical double layers. The description of nanoparticle interaction was carried out in the framework of the DLVO theory under the condition of the Poisson-Boltzmann equation linearization. The developed phenomenological charge regulation model, based on the assumption that a nanoparticle can be substituted with its equivalent screened point charge, was used to create an original method of modifying the linear superposition approximation (MLSA method), which allows to determine the potential energy of a system of many interacting colloidal nanoparticles.

The developed colloid nanoparticle interaction model provides qualitative agreement with experiment in describing the initial stage of coagulation; for the systems satisfying the limit of applicability it does not impose any restrictions on the number of interacting particles and thus allows to simulate the processes of formation and interaction of nano aggregates, while predicting the presence of orientation effects, which may cause the formation of clusters of different morphologies.

It should also be noted that in order to determine the potential energy of interaction for a given spatial configuration of nanoparticles the MLSA method only requires solving the system of linear algebraic equations with $m \times m$ matrix, where $m$ is the number of interacting particles. This implies the relative simplicity of the method and the possibility of its smooth integration into further numerical or analytical modeling of nanoparticle coagulation dynamics.

References
