Non-equilibrium Ionic Assemblies of Oppositely Charged Nanoparticles

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We implemented a kinetic Monte Carlo simulation scheme to perform the first detailed study of the structure and evolution kinetics of non-equilibrium ionic assemblies formed in solutions of oppositely charged nanoparticles. A wide range of dynamic selfassembled aggregate configurations were found, including crystalline/fibril-like/ disordered clusters and network-like gels. The solution conditions (particle charge, temperature, ionic strength, etc.) under which a specific aggregate structure can be realized were determined by simulations. The dynamic ionic assemblies hold great promise in a variety of emerging applications such as templated polymerization of charged molecules and assembly of charged nanoobjects.



crystalline cluster

fibril-like cluster





disordered cluster

network-like gel

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