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Strong ion-driven depletion causes Nano-particle assembly YAOHUA LI, JAIME MILLAN, MENG SHEN, TRUNG NGUYEN, MONICA OLVERA, Northwestern Univ — Ion mediated interaction between Nanoparticles (NPs) have been extensively utilized in experiments such as protein crystallization. At high ionic concentration, strongly correlated ions can form short chains which induce depletion-type attraction between charge or non-charged nanoparticles. In this regime, previous theoretical and numerical efforts such as DLVO theory or the primitive model breaks down because they either neglect excluded volume of ions or solvent-induced correlation like hydration effects, which have non-trivial contribution to NP-NP interactions. To include these effects, we perform multi-scale molecular dynamics simulation to obtain the potential of mean-force between NPs immersed in 0.3M-3M NaCl solution. Ion pair potentials that reproduce radial distribution function from atomistic simulation are derived and used for implicit solvent simulation. The attractive interaction between NPs is of order of several kT (thermo energy) and scales with NP size and ionic strength. The functional form of the potential matches with classical depletion theory. Our results suggest that ion-induced depletion dominate interaction between NPs at high ionic strength.

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