Cluster Formation by Charged Nanoparticles on a Surface in Aqueous Solution

Dongsheng Zhang, Pedro Gonzalez-Mozuelos, Monica Olvera de la Cruz

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Dispersion forces due to the presence of water are most important in determining the solubility of macroions and charged nanoparticles in ionic solutions. The effective pair potentials between ions and nanoparticles was calculated by using an integral-equation model that includes the water explicitly. By using the SPC/E model for water, the short-range pair interaction between nanoparticles was found to be similar to the Lennard Jones potential but with a sharper decay and a strong attractive well (of the order of -12KT for 3 nm radius nanoparticles). **[Fig 1]** Molecular dynamics simulations were then used to study the phase behavior of nanoparticles on a surface in aqueous solutions. The nanoparticles with small charges form nanoclusters with high degree of ordering, **[Fig 2]** while nanoparticles with large degree of charge do not. **[Fig 3]** Our results also showed that the charge renormalization depends on the charges of nanoparticles as well as the size of the nanocluster to which the nanoparticles belong.

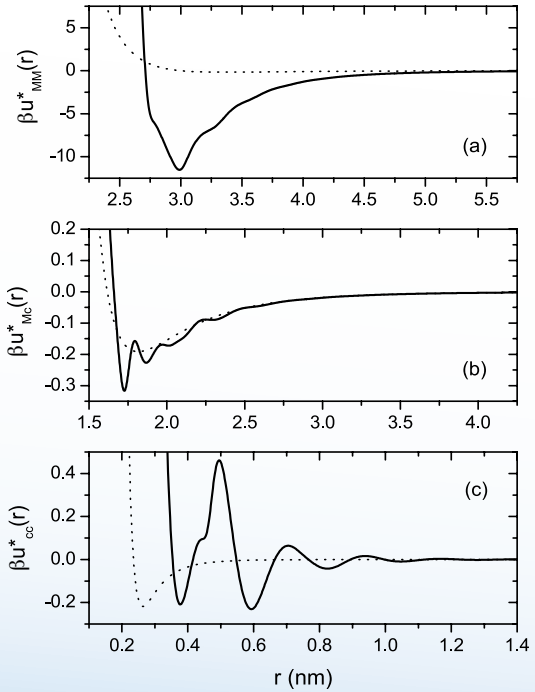

Fig. 1. *The short-range component of the effective pair potentials among the ions at infinite ionic dilution (solid lines) and the corresponding Lennard-Jones potentials (dotted lines) [nanoparticle-nanoparticle (a), nanoparticle-counterion (b), counterion-counterion (c)].*

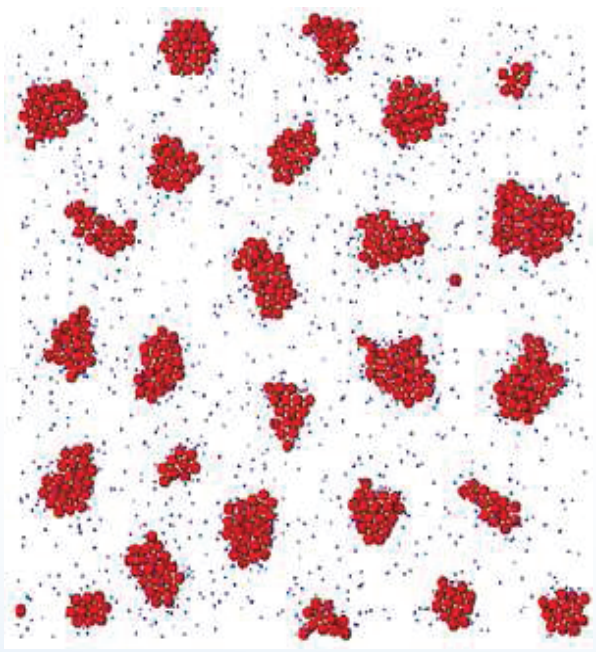

Fig. 2. *Snapshots from MD simulations for nanoparticles (qM=-3) and counterions (q=1) in solution confined to a plane The red dots represent the nanoparticles while the blue ones represent the counterions. These figures were prepared using VMD.*

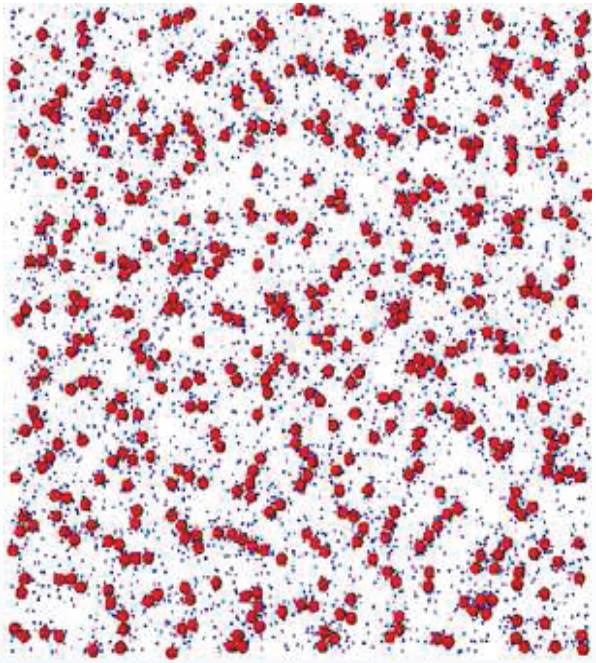

Fig. 3. *Snapshots from MD simulations for nanoparticles (qM=-8) and counterions (q=1) in solution confined to a plane The red dots represent the nanoparticles while the blue ones represent the counterions. These figures were prepared using VMD.*

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