Numerical simulation of the nanosized particle aggregation near the electrode using the Poisson-Nernst-Planck equations in a closed system

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The phenomenon of clustering of microsized latex particles in the vicinity of the electrode was explained by the model of electroosmotic flow. However, nanosized gold particles are aggregated onto carbon-coated copper grids under a low electric potential, which is not high enough to make electric current. The model cannot explain the nonosized particle aggregation in the vicinity of the electrode under such a low voltage. Therefore, Poisson-Nernst-Planck equations including mass balace constraints for each ions are used to explicitly solve the distribution of electric potential between electrode and two nanosized particles because the charateristic scale of length - the radius of particle, a is not much larger than the Debye length in the case of the nanosized particle. Electrostatic repulsion barrier between two particles is smaller than that obtained from the generic Poisson-Boltzmann equation. In addition, Van der Waals attraction and Brownian motion are considered in the simulation. The results of the simulation explain that nanosized particles are aggregated or dispersed in the vicinity of the electrode according to the material of particles.