Computer modeling and simulation of electrically charged nano/micro-particles interaction into aqueous solution by the Brownian dissipative dynamics of their atomic counterions ensemble

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On the basis of free energy functional of charged ions and equation of diffusion of ions in self-consistent electric potential, an original method of Brownian dissipative dynamics of ions near electrically charged colloidal micro/nano-particles in aqueous solution or dusty plasma particles in the air is proposed for investigation of ionic atmosphere structure near charged surfaces, and electric interparticle force is calculated ($a<<R$, $|Q|<<|q|$, where a and q are radius and charge of small ion, R and Q are radius and charge of micro/nano-particle).

The average stationary displacement of ions obtained from this method is agreed with the Poisson-Boltzmann (PB) equation. The additional information which is not included in PB equation is the fluctuations of ionic concentration and interparticle force. The dependence of electrostatic energy and entropy of such a system on the distance between the centers of the nanoparticles is determined in the numerical experiments. The obtained results in connection with the ordinary Derjaguin-Landau-Verwey-Overbeek theory and other similar models are considered.