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Reactive Monte Carlo Simulation for Colloidal Particles

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Abstract: We use a reactive Monte Carlo simulation method [1] and the primitive model of electrolyte to study acid-base equilibrium that controls charge regulation in colloidal systems. The simulations are performed in a semi-grand canonical ensemble [2], in which colloidal suspension is in contact with a reservoir of salt and strong acid. The interior of colloidal particles is modeled as a low dielectric medium, different from the surrounding water. The effective colloidal charge is calculated for different number of surface acidic groups, pH, salt concentrations, and types of electrolyte. In the case of potassium chloride the titration curves are compared with the the experimental measurements obtained using potentiometric titration.

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References:

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[2] M. Lund and B. Jönsson, Q. Rev. Biophys. **46**, 265 (2013).