Electrophoresis of Highly Charged colloids.

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Abstract : The motion of a charged colloidal particle in an electric field is an extremely interesting problem due to the complex interplay between electrostatic, thermal and viscous forces in determining its motion. Using computer simulations, we study the electrophoretic motion of a positively charged colloid (macroion) in an electrolyte solution in the framework of the primitive model. In this model, the electrolyte is considered as a system of negatively and positively charged microions (counterions and coions, respectively) that are immersed into a structureless medium. **Hydrodynamic interactions** are fully taken into account by applying a hybrid simulation scheme, where the charged ions (i.e. macroion and electrolyte), propagated via molecular dynamics (MD), are coupled to a Lattice Boltzmann (LB) fluid. In a recent electrophoretic experiment by Martin-Molina *et al.* [J. Phys. Chem. B **106**, 6881 (2002)], it was shown that, for multivalent salt ions, the mobility μ initially increases with charge density σ, reaches a maximum and then decreases with further increase of σ. The aim of the present work is to elucidate the behaviour of μ at high values of σ.

The role of hydrodynamic-interactions is inferred from direct comparisons to Langevin simulations where the coupling to the LB fluid is switched off. Langevin simulations can give qualitatively different results from simulations with hydrodynamic coupling for low values of bare colloid charge Q.

References

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