

Abstract Submitted
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A Mesoscale Simulation Method for High Salt Concentrations

STEFAN MEDINA¹, Caltech, USA / University of Mainz, Germany, FRIEDERIKE SCHMID, University of Mainz, Germany — In mesoscale simulations of electrolyte solutions the interplay between electrostatics and hydrodynamics plays the critical role for computational efficiency and accuracy. In the past it became apparent that high salt concentrations are too costly, if every salt ion is treated explicitly as a separate particle. On the other hand, charges are highly screened at high salt concentrations and ion-ion correlations are less important than in the low-salt limit. Therefore, we have developed a dynamic mean-field treatment of charges which is expected to be perfectly sufficient in many cases leading to applications in controlled manipulation of polyelectrolytes and charged colloids by external electric fields.

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