Calculation of effective interaction between like-charged particles ; Integral equation theory of liquids and Monte Carlo simulation

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Abstract

Acidic proteins, which are negatively charged particles, show an interesting condensation behavior in an electrolyte solution if the electrolyte has multivalent cations[1]. As the electrolyte concentration increases, the state changes in order of dispersion, condensation, and re-dispersion. So, the effective interaction changes repulsive, attractive, and repulsive, in other words, an effective attraction between like-charged particles exhibits reentrant behavior to the electrolyte concentration. DNA also shows this behavior.

In our previous study, to explain this phenomenon, we calculated the effective interaction between anions by using the OZ-HNC theory, which is one of the integral equation theories of liquids[2]. These results reproduced the above experimental results qualitatively. We should note that the results given by the integral equation theory are based on an approximation, namely the HNC approximation. The confirmation using molecular simulation is important.
However, it is difficult that the concentration dependence of effective interaction is investigated by simulation. It is one of the results that the reentrant behavior had been reproduced by molecular simulations. Thus, we decided calculation parameters based on the results of HNC-OZ theory. And we calculate the effective interaction between anions by using the Monte Carlo simulation in the present study.

We carried out the modeling using the results of the OZ-HNC theory to survey the reentrant behavior. Here, we prepared the electrolyte solution which includes monovalent anion and multivalent cation. Additionally, in this system which strong coulomb interaction works, we predicted easy to fall into the local minimum. As a measure, we calculated with replica exchange method.

Some of the results are shown in Figure 1. The effective attraction of the OZ-HNC theory was a lot larger than simulation when the electrolyte concentration was low. So, the results of the OZ-HNC theory and simulation were different quantitatively because the OZ-HNC theory provides larger effective attraction. On the other hand, the simulation results indicated the reentrant behavior to the concentration. So, the results of the theory and simulation were qualitatively same. And these results indicated the HNC approximation emphasizes an effect of the mediation site between like-charged particles.

REFERENCES

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FIGURES

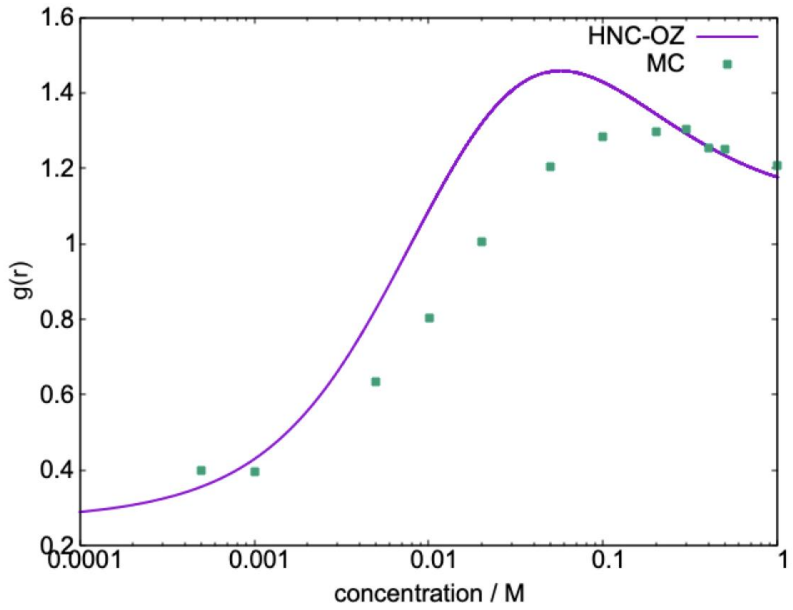

Figure 1: Anion-concentration dependence of the values of radial distribution function g(r) at a specified separation. The corresponding separations are 5.38 $\mathrm{\AA}$ and 5.60 $\mathrm{\AA}$ for the HNC-OZ theory and MC simulation, respectively.