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Molecular dynamics study on the viscosity of aqueous solutions

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Introduction

One of the classical areas of study in physical chemistry is the effect of ions in an aqueous solution and their dependence on the ionic properties, which have significant roles on the dynamic behavior of the medium and so on its viscosity. Viscosity of electrolyte solutions is of considerable interest due to its importance in numerous industrial systems, especially those involving electrochemical processes. Thus, in this investigation, we have explored the accuracy with which the viscosity of simple ionic systems can be computed through falling-ball method using molecular dynamics simulations, with the ultimate goal to extend these simulations to more complex and/or industrially relevant systems.

Method

A viscosity evaluation program based on our integrated classical molecular dynamics program "New-RYUDO" has been developed in our laboratory. A characteristic cubic model with the inserted viscosity measurement ball has been used for the viscosity evaluation (Fig. 1). The models included 272 water molecules, of which the density was set to 0.99 g/cm^3 at 298.15 K and 100 kPa, and cations were added at different amounts for further viscosity calculations of electrolyte.

Principles of falling-ball method have been used for the viscosity evaluation for electrolyte system, where the coefficient of viscosity (μ) is defined as

$$\mu = \frac{F}{3\pi D_p \zeta u_t}$$

Here F is the force on the ball, D_p is the diameter of measurement ball, ζ is the correction coefficient and u_t is the subsidence speed of the ball. The calculations were performed for 50,000 steps with a time interval of 0.1 fs.

Results and Discussion

A constant force, 1.2x10^{-9} N, is applied to the viscosity measurement ball at x-direction. Thus, it moves compulsorily in the system, of which the trajectory in bulk water is shown in Fig.1. The speed of the measurement ball can be derived from the moved distance during the simulation, that for bulk water is seen in Fig.2. Therefore, the viscosity for water is calculated as 1.042 mPa.s at 298 K, which is very close to the experimental value (1.002 mPa.s). Further viscosity calculations have been performed for electrolytes of Li, Na, K and Cs at their different concentrations and the results are also in good agreement with experimental ones. Viscosity analysis will be useful to understand the dynamical behaviors of simple ions in aqueous solution.

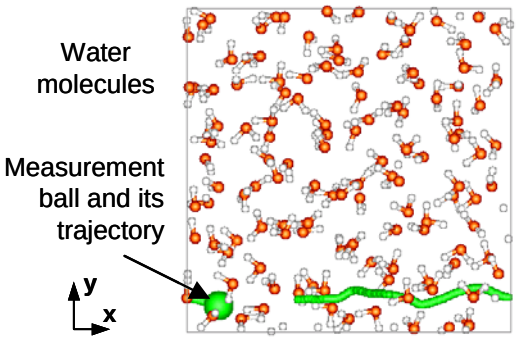

Fig.1. Trajectory of the viscosity measurement ball in water molecules

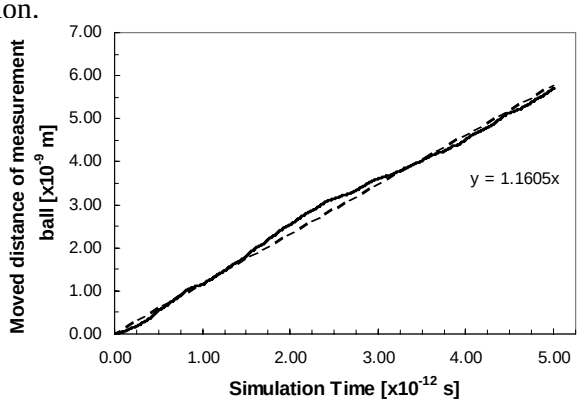

Fig.2. Moved distance of the viscosity measurement ball in water during the MD simulation. Slope gives the speed of the ball.