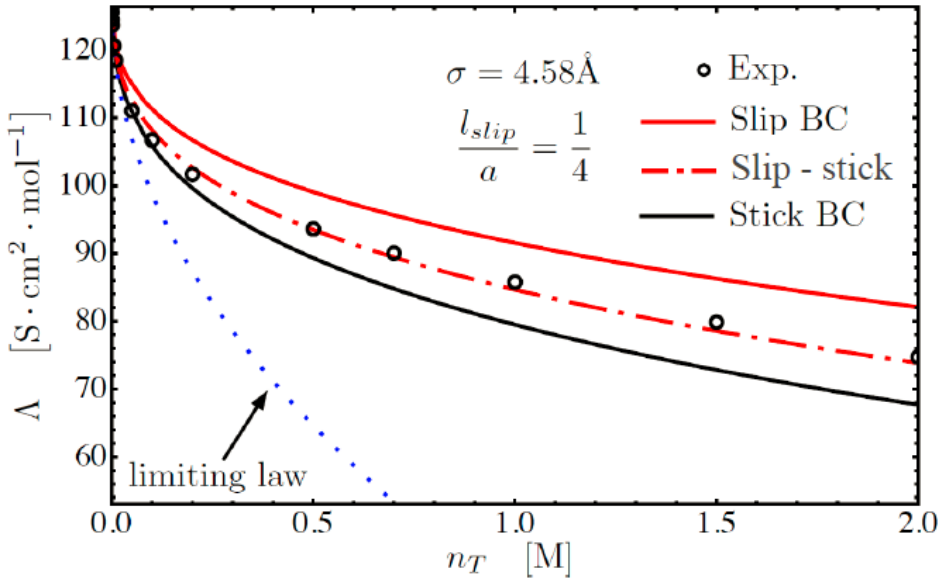
Conductivity and Viscosity of Electrolyte Solutions

G. Nägele

in collaboration with C. Contreras-Aburto, University of Guanajuato, Mexico

We have derived a unifying mode-coupling theory (MCT) method of calculating linear transport properties of concentrated strong electrolyte solutions [1-4]. The ions are described on a primitive model level as uniformly charged hard spheres embedded in a Newtonian fluid characterized by its dielectric constant and shear viscosity. The Brownian dynamics of the ions is described by the multicomponent generalized Smoluchowksi equation. For the first time, the salient hydrodynamic interactions between the ions are accounted for both regarding the short-time electro-osmotic flow effect appearing in conduction and electrophoresis, and the long-time relaxation effect related to the dynamics of the electric double layer surrounding each ion. The predictions by the method for the electrolyte conductivity Λ (see figure taken from [2]) and the reduced steady-shear viscosity, as functions of the total ion concentration, n_T, are in good agreement with experimental data for aqueous sodium chloride solutions.



In collaboration with C. Contreras-Aburto and R. Castaneda-Priego (U. of Guanajuato, Mexico) and M. Heinen (Düsseldorf University), molecular dynamics and modified hypernetted chain approximation calculations are performed presently for size- and charge asymmetric electrolyte solutions. The pair distribution functions obtained by these two methods will be used as input to our planned MCT calculations of transport properties of asymmetric electrolytes with significant ion pairing and non-linear electrostatic screening tendencies.

[1] C. Contreras-Aburto and G. Nägele, J. Chem. Phys. **139**, 134109 (2013).

[2] C. Contreras-Aburto and G. Nägele, J. Chem. Phys. **139**, 134110 (2013).

[3] C. Contreras-Aburto and G. Nägele, J. J. Phys.: Condens. Matter **24**, 464109 (2012).

[4] G. Nägele, M. Heinen, A.J. Banchio, and C. Contreras-Aburto, Eur. Phys. J. Special Topics **222**, 2855 (2013).