

Modeling of specific ion effects: Molecular dynamics and integral equation theory

Luboš Vrbka

Institut für Theoretische und Physikalische Chemie
Universität Regensburg

`lubos.vrbka@chemie.uni-regensburg.de`

In the last several years, the so called specific ion effects have received a lot of attention. In my talk, I will present our simulation results concerning ions at the air/water interface and in protein solutions, and also our experience with integral equation theory as a promising tool for qualitative and quantitative description and prediction of bulk properties of electrolyte solutions.

First, the different propensity of various atomic and molecular ions for the air/water interface will be presented. Although our findings seem to contradict the classical textbook knowledge (Onsager-Samaras theory of electrolytes, Gibbs adsorption isotherm), closer inspection reveals that this is (at least partially) not the case. This issue will be thoroughly discussed.

Second part of my presentation will be devoted to our computer simulations of ion – protein interactions. Using two different problems – namely the preference of sodium over potassium in the vicinity of proteins, and the effect of salts on enzymatic activity of horseradish peroxidase – I will show that the usage of 'averaged' protein models is highly questionable, due to the importance of individual ion – aminoacid interactions.

In the last part of the talk, the usage of statistical mechanics and liquid state theory (integral equations) for description of bulk electrolyte properties will be discussed. By using potentials of mean force coming from molecular dynamics simulations as inputs in the theory, we are able to interconnect calculations on atomic level, statistical thermodynamics, and experiment, providing thus a unified picture of ions in solution. The other possibility lies in employing simple parameters coming from *ab-initio* calculations, and combining these with 'chemical feeling' of ion hydration.