

Modeling of specific ion effects using MD simulations and integral equation theory

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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 and ice/water interfaces 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 complex electrolyte solutions.

In the beginning, the reasons behind 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 not the case. Our results of simulations of the effect of salt on water freezing will be also briefly discussed.

Second part of my presentation will be devoted to our studies of ion–protein interactions. Using the example of the preference of sodium over potassium in the vicinity of proteins, 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.