Ions at the Protein/Water and Ice/Water Interfaces - A Molecular Dynamics Study

Luboš Vrbka

Institut für Theoretische und Physikalische Chemie
Universität Regensburg

lubos.vrbka@chemie.uni-regensburg.de

In the last several years the behavior of ions with respect to the air/water interface has received much attention. We extended these studies also to the surfaces of solvated proteins and to the ice/water interface.

First, we studied by MD simulations preferential adsorption of choline, sodium, chloride, and sulfate to protein surfaces. The salt–induced change of the protein activity observed experimentally for HRP protein could be ascribed to specific local pairing of ions with amino acid residues in the vicinity of the active site.

Second, we aimed at understanding why sodium cations are preferred over potassium in the vicinity of protein surfaces. The interaction behind this biologically extremely relevant phenomenon is again very specific. The binding of these cations to proteins happens via pairing with carboxylate groups of Asp and Glu amino acids.

Our results indicate, that the use of simplified protein models is highly questionable, since the ion–protein interactions are highly specific. The 'averaged' protein models, therefore, do not provide enough details on atomic level to properly describe the local character of such interactions.

The atmospherically and technologically very important process of brine rejection from freezing salt solutions was investigated using atomistic MD simulations. The calculations allowed to propose a microscopic mechanism of brine rejection, in which a fluctuation (reduction) of the ion density in the vicinity of the ice front is followed by the growth of a new ice layer. Presence of salt slows down the freezing process, which leads to the formation of an almost neat ice next to a disordered brine layer.