1 Abstract in English

The present thesis consists of ten publications[1–10] in international peer–reviewed journals with an extended introduction and a detailed discussion of the content of these papers. The work can be divided into three different topics, with ion behavior at interfaces being the common denominator. Namely, we focused on the following three issues:

- Ions at the air/water interface
  We discuss the fact that certain inorganic ions can (contrary to the textbook knowledge) exhibit a propensity for the air/water interface. This is particularly true for large polarizable anions, such as heavier halides, azide, or thiocyanate. Cations with aliphatic chains also show affinity to the surface, however, due to different reason – their hydrophobicity. The interplay between hydration and polarization forces in complex ionic mixtures is discussed in detail in this part of the thesis.

- Ions at the ice/water interface
  Brine rejection from freezing salt solutions (*e.g.*, sea water) is a very important natural phenomenon influencing the global climate. Molecular details of this process are established using molecular dynamics simulations.

- Ions at the protein/water interface
  We studied specific ion–protein interactions. First, we discuss the possible reasons behind the salt induced superactivity in horseradish peroxidase. Second, we present rationalization and quantification of the fact that sodium si preferred over potassium at protein surfaces.

Most of the work has been done using molecular dynamics (MD) simulations. When needed, also other methods of computational chemistry were used (*e.g.*, quantum mechanical methods were employed during the development of interaction potentials for some molecules and ions). Frequently, we report a results of joint theoretical and experimental research. The discussion of the experimental methods is beyond the scope of this thesis, however, the experimental findings are briefly discussed to demonstrate the relevance of our results in a wider context.