

## Interactions between ions and proteins in water: The Hofmeister series

**Pavel Jungwirth**

*Academy of Sciences of the Czech Republic*

*and Center for Complex Molecular Systems and Biomolecules,*

*Flemingovo nám. 2, 16610 Prague 6, Czech Republic*

In 1888 Hofmeister discovered a series of salt ions that have consistent effects on the solubility of proteins and (as was discovered later) on the stability of their secondary and tertiary structures, which is crucial also for their biological function. More 100 years after its discovery, we are only starting to fully understand the microscopic mechanisms behind the Hofmeister series.

By means of molecular dynamics simulations we quantify affinities of ions to building blocks of proteins in water. We critically examine the suitability of dielectric models for the description of the protein/water interface in analogy to the water/vapor interface. Little correlation is found between these two interfaces in terms of ion segregation. Therefore, a local picture of pairing of ions from the solution with charged and polar groups at the protein surface is advocated and combined with a model for segregation of large soft ions at hydrophobic patches of the protein surface.

