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Editorial

# Editorial for special issue on ions

Small ions, by virtue of the strong electrostatic interaction, constitute a key component in many complex physical, chemical and biological systems. Recent years have seen tremendous progress in probing the way ions are involved in such systems. Experimental methods have been refined to probe the structure and dynamics of ions in bulk systems and microenvironments. Computer simulations of detailed models of molecular systems are now an integral part of the process of investigating these complex systems. Molecular dynamics (MD) simulations of large molecular systems based on empirical force fields, or even accounting for electronic degrees of freedom explicitly using *ab initio* molecular dynamics (AIMD), have become increasingly feasible. Studies of biological channels, in particular, have now reached a culminating point with the determination of the first high-resolution crystallographic structure of biological potassium-selective channel, the KcsA channel from *Streptomyces lividans*.

The idea of a Special Issue on "Ions in Complex Physical, Chemical and Biological Systems" arose from a Symposium of the American Chemical Society meeting held in Washington, DC, in September 2005. Most of the authors who participated in the ACS Symposium have gracefully accepted to contribute to the Special Issue. The great variety of subjects covered testifies to the importance of ions in a wide range of complex systems and to the talent and creativity of the authors. These exciting contributions provide a rich cross-section illustrating this vast field. We are also particularly grateful to Alan Cooper, the Editor of *Biophysical Chemistry*, for his help and support in preparing this Special Issue.

The first three articles are concerned with experimental and theoretical approaches for the determination of the hydration structure of ionic aqueous solutions. These approaches are important as they allow one to gain access to detailed information such as the number and the orientation of water molecules located in the hydration shell of an ion, information of paramount importance in all considerations about more complex physical, chemical and biological systems. The first article, by Ansell et al., provides a timely review of the state-of-the-art in X-ray and neutron scattering experiments for the determination of the hydration structure of ions in aqueous solutions. Their article explains how the 'difference' methods of Neutron Diffraction with Isotopic Substitution (NDIS), and Anomalous X-ray Diffraction (AXD), can be used to obtain direct information regarding the radial pair distribution functions of many cations and anions in solution. This is followed by an article from Soper and Weckström that presents new diffraction results on the hydration structure of potassium halide ions in water, interpreted with the method of empirical potential structure refinement. In the third article, by Varma and Rempe, published experimental and theoretical data are analyzed for the first three alkali metal ions, along with new results from *ab initio* molecular dynamics and the experimental results from the previous articles. The analysis shows a consistent, but surprising picture of the structures of the first hydration shells of $Li^+$, $Na^+$, and $K^+$ ions.

Important manifestations of solvation and the role of ions as an organizational factor in supramolecular chemistry are reflected in bulk thermodynamic properties. The volumetric properties of electrolytes in solutions and their relation to the interactions of the constituent ions with their environment are discussed in an article from Marcus. The role of dispersive (non-electrostatic) forces in Hofmeister effects is discussed by Nostro et al. The impact of ionic strength on the stability and characteristics of a DNA Holliday Junction Switch is discussed by Mount et al. Computational results on the hydration structures and electronic properties of the formohydroxamate anion in liquid water from AIMD are discussed by Leung.

Studies of ions in complex non-isotropic physical environments are exemplified with studies of microsolvated ions in water clusters, by Broendsted and Andersen, ions at the air/water interface, by Hrobarik et al., and ions in nanopores by Saint-Martin et al. The subject of ions in the confined environment of narrow pores leads naturally to the study biological transmembrane ion channels. Ion channels are specialized proteins forming passive pores embedded into the cellular membrane. Their function is to provide a selective and energetically favorable pathway for ions movements across the membrane. The gramicidin channel, one of the simplest and best characterized transmembrane molecular pores, is a great model system to try and understand the fundamental principles governing ions in the confined environment of a narrow molecular pore. The gramicidin channel is the subject of two articles. Allen et al. discuss the energetic factors controlling the permeation of ions using molecular dynamics simulations with free energy potential of mean force (PMF) techniques, and Mamonov et al. discuss the dissipative factors, mobility and diffusion constant of potassium ion. The gramicidin channel

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displays some specificity for cations, but is otherwise not very selective. The structure of the KcsA channel, a highly selective channel, gave a fresh impetus to the efforts aimed at gaining insights into the mechanism of ion permeation through a biological selective channel. This is illustrated by two contributions. Noskov and Roux review and discuss the historical views of ion selectivity spanning the last 50 years in the context of recent work on the KcsA channel. This is followed by the final contribution, an investigation by Bucher et al. on the importance of polarization effects and charge transfer in the narrow selectivity filter of KcsA using AIMD.

Susan Rempe
*Sandia National Laboratories, USA*
*E-mail address:* SLRempe@sandia.gov.

Benoit Roux
*University of Chicago, USA*
*E-mail address:* roux@uchicago.edu.
Corresponding author.

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