WATER IN BIOLOGICAL AND CHEMICAL PROCESSES

Building up from microscopic basics to observed complex functions, this insightful monograph explains and describes how the unique molecular properties of water give rise to its structural and dynamical behavior, which in turn translates into its role in biological and chemical processes.

The discussion of the biological functions of water details not only the stabilizing effect of water in proteins and DNA, but also the direct role that water molecules themselves play in biochemical processes, such as enzyme kinetics, protein synthesis, and drug–DNA interaction. The overview of the behavior of water in chemical systems discusses hydrophilic, hydrophobic, and amphiphilic effects, as well as the interactions of water with micelles, reverse micelles, microemulsions, and carbon nanotubes.

Supported by extensive experimental and computer simulation data, highlighting many of the recent advances in the study of water in complex systems, this is an ideal resource for anyone studying water at the molecular level.

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Cambridge Molecular Science

As we move further into the twenty-first century, chemistry is positioning itself as the central science. Its subject matter, atoms and the bonds between them, is now central to so many of the life sciences on the one hand, as biological chemistry brings the subject to the atomic level, and to condensed matter and molecular physics on the other. Developments in quantum chemistry and in statistical mechanics have also created a fruitful overlap with mathematics and theoretical physics. Consequently, boundaries between chemistry and other traditional sciences are fading and the term *Molecular Science* now describes this vibrant area of research.

Molecular science has made giant strides in recent years. Bolstered by both instrumental and theoretical developments, it covers the temporal scale down to femtoseconds, a timescale sufficient to define atomic dynamics with precision, and the spatial scale down to a small fraction of an angstrom. This has led to a very sophisticated level of understanding of the properties of small molecule systems, but there has also been a remarkable series of developments in more complex systems. These include protein engineering, surfaces and interfaces, polymers, colloids, and biophysical chemistry. This series provides a vehicle for the publication of advanced textbooks and monographs introducing and reviewing these exciting developments.

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From Structure and Dynamics to Function

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"To my mother and my father, Abha and Binay K. Bagchi. They taught me, from an early age, to love poetry and science, opening doors to the wonders of Nature."

"Understanding the role of water as the ubiquitous solvent for the chemical biology and throughout molecular science remains one of the most active areas of current scientific research. The puzzling issues that arise throughout this field require a unified understanding of structure, dynamics and thermodynamics. This book provides a valuable resource in relating microscopic properties to complex phenomenology, connecting diverse topics of contemporary interest."

David J. Wales, University of Cambridge

"This book by Biman Bagchi covers an extremely broad range of topics on water, written with an eye to relating theory and experiment and by someone who has insight into both. Its use of recent references in the field is a helpful attribute. The author emphasizes that our understanding is not a closed subject and so there will be further room for developments, debate on interpretation, and discussions. For teachers of topics in equilibrium and nonequlibrium statistical mechanics there is also, I believe, much useful material on interesting applications."

Rudy A. Marcus, California Institute of Technology

"Water continues to both fascinate and confound those who study its properties and its vital roles in life's structures and dynamical processes. In this unique book Biman Bagchi has brought together an extraordinary range of experimental data and the results of both theory and simulation studies at a level generally accessible to readers with a background in chemistry at the first year university level. He illuminates how the remarkable properties of water are key to a multitude of chemical and biological processes and in doing so provides both insight and the springboard for new investigations of this endlessly fascinating liquid."

Graham R. Fleming, University of California, Berkeley

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The color plates will be found between pages 78 and 79.

Preface

This book attempts to summarize the large body of experimental and simulation data gathered recently on the structural and dynamic aspects of water in complex chemical and biological systems. In the process we try to present a unified view of this emerging field. While most discussions on water focus on its role in complex systems (like the role of water as a polar solvent stabilizing the native state of a protein), I thought it would be equally, if not more, appropriate to study and if possible explain why water has so many unique properties and how it is able to play important parts in so many diverse settings. For example, water molecules themselves need to change and adjust to the surface. In enzyme catalysis, they participate actively and get consumed *as a chemical – not act just as a good solvent facilitating the catalysis* – a fact not often appreciated.

Many important aspects of water have been discovered only in the last two decades or so. For example, we came to know about the astonishingly fast rate of solvation of a polar solute by water only around the mid-nineteen nineties! The detailed role of water in chemical reactions, such as in electron transfer, has also become clearer around the same time. It is therefore not surprising that it is only now that we have turned our attention towards understanding molecular aspects of water's role in biology. The specific role of water in most of the biological processes is far from well understood even today.

Studies of unique properties of water have often followed two disjointed paths. On the one side, detailed microscopic properties of water molecules, both in the bulk and in and around biomolecules, have been studied in vitro, such as water structure and arrangement around proteins and DNA. These studies have often remained confined to their own domains of choice/focus, with hardly any attempt to connect it with other properties and functions of water. The second line of studies has focused on the utilitarian aspects of water. Here the approach is largely qualitative and focused on the role of water in various aspects of life and nature. The latter have been popular since antiquity. Neither of these two approaches addresses the explicit (especially dynamic) role of water molecules in biological functions.

Water that is present in biological cells, in the grooves of DNA, on the surfaces of proteins is found to be quite different from water in the bulk, the water that we drink. The term “biological water” was coined to highlight this difference. In nature, water is also found within rocks and confined systems, such as in tree leaves. Such confined water also exhibits properties quite distinct from those in the bulk. The main modification that occurs from the bulk state of water is the partial or even full loss of the hydrogen-bond network that so uniquely defines water. In biological and many natural systems, water faces a multitude of interactions from the surface. However, water seems to retain sufficient resources of its own to adjust to new environments and continue to perform its wide-ranging roles.

We have placed special emphasis on properties that have been observed in biomolecules, such as proteins, DNA, and RNA, and in other complex systems such as micelles, reverse micelles, and carbon nanotubes. As observed above, we tried to see what happens to water due to the proximity to a foreign surface. Second, we attempted to provide a coherent explanation of properties observed from a modern, *molecular*, *often dynamic*, *perspective*. The latter relies heavily on recent advances in the field, often driven by computer simulations. Third, we spend considerable effort to discuss biological functions of water. By “biological function” we do not imply only the stabilizing effect of water in proteins and DNA, but the direct role that water molecules themselves play in biochemical processes, such as in enzyme kinetics and protein synthesis, that are essential for life. Thus, the third purpose of this book is to articulate such biological and chemical functions in the light of our current understanding of molecular aspects of water although, as stated above, the development in this area is largely incomplete.

Throughout the monograph, we have attempted to avoid using mathematical expressions and minute details of sophisticated theories in order to make the content accessible to a larger number of students and interested readers who are not professional researchers in the area. We believe that the properties of water are so interesting, especially given the uniqueness of the liquid, that many scientifically inclined people will find the subject fascinating. Although in some places detailed discussions have been included to give a flavor of the subject, we have attempted to keep them at a minimum. We also address, towards the end of the book, certain advanced topics of current research in water. They are not disjoint from the earlier chapters and substantiate our efforts to explain the uniqueness of water. But readers, if not interested in advanced topics, can avoid these chapters without much loss to the completeness.

Our focus on molecular explanations of the observed properties distinguishes the present monograph from the others existing in the literature. At the same time, this approach also limits the range of topics that we could address here. But there are many excellent books/monographs on water which can supplement this lacuna.

Da Vinci called water “Natural vehicle of change”. We attempt to show here that the detailed role of water in biological and chemical change can be fascinating and elusive at the same time. We hope this book (despite many lacunae) will be welcomed by students and scientists at large, especially because it documents some of the significant progress that has been made in the last few decades.

It is fitting to end the preface of this book on water with the following well-known quote of Mark Twain. “My books are like water; those of great geniuses are like wine. (Fortunately) everybody drinks water.” I hope this book on water qualifies as Mark Twain’s water.

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