Preface

Molecular modeling has seen great progress in a wide range of biological applications in recent years due to the advancement of novel algorithms and high-performance computing. The gap between the timescales achievable by experiments and by computer simulations has been significantly reduced due to the concurrent advances in both experimental and theoretical techniques. Scientists can nowadays access microsecond-to-millisecond timescales with atomic detail, which is sufficient to characterize many important biological processes, such as the folding dynamics of some key proteins. This book captures the perspectives of leading experts on this transformation in theoretical molecular biology and illustrates how molecular modeling approaches are being applied to change our understanding of many important aspects of structural and molecular biology. Together, I hope these chapters provide a comprehensive overview of the fundamentals of molecular modeling and its applications in modern quantitative biology.

Although molecular modeling has been around for a while, the groundbreaking advancement of massively parallel supercomputers and novel algorithms for parallelization is shaping this field into an exciting new area. There is an increased interest in molecular modeling, as witnessed by many new conferences and newcomers, particularly from the emerging world. Until now progresses, particularly the development of novel algorithms and massively parallel computing techniques, have been led by a small group of risk-takers. With the maturation of these algorithms and simulation techniques, a broadly accessible book that lays out the fundamentals of molecular modeling will helpfully broaden these techniques to a much larger community.

This book covers both the advanced techniques of molecular modeling and the latest research advancements in biomolecular applications from leading experts, so the content should be of interest to academic and industry professionals in addition to graduate students. The book begins with a brief introduction (preface) of the major methods and applications that are presented in the chapters for molecular modeling and its applications in structural and molecular biology. Section I: Advanced Simulation Techniques (Chapters 1 through 3) covers the development of cutting-edge methods/algorithms, new polarizable force fields, and massively parallel computing techniques. Chapters 4 through 12 will describe how these novel techniques can be applied in various research areas in molecular biology. Section II: Self-Assembly of Biomolecules (Chapters 4 through 7) covers topics related to the self-assembly of biomacromolecules, including protein folding, RNA folding, amyloid peptide aggregation, and membrane lipid bilayer formation. Section III: Biomolecular Interactions (Chapters 8 through 10) focuses on the important biomolecular interactions, including protein interactions with DNA/RNA, membrane, ligands, and nanoparticles. Section IV: More Applications in Molecular Biology (Chapters 11 and 12) covers other emerging topics in biomolecular modeling, such as DNA sequencing with solid-state nanopores, biological water under nanoconfinement, and so on.

This book provides advanced techniques and real-world examples, which should be useful to senior undergraduate and graduate students, as well as established researchers in chemistry, molecular biology, computer science, and bioengineering. I hope courses such as computational chemistry, biophysical chemistry, biophysics, statistical mechanics, and computational molecular biology might find some of the contents useful as textbook or supplementary material. In addition, it might be of interest to academic and industry professionals in drug discovery and other biotechnologies.

Finally, I thank all the contributing authors for their excellent work and fruitful collaboration on this project. The very helpful and efficient technical assistance of Luna Han in putting together this book in a timely manner is greatly appreciated.

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