

"This book is a state-of-the-art report on the description of molecular energetics using force fields, which are the most critical element in computer simulations of biomolecular systems. The 16 chapters, written by leaders in the field, provide in-depth reports on all important current issues, including the representation of polarization, quantum mechanics-based force fields, and coarse-grained approaches for RNA, DNA, and membranes. This is an important reference for anyone involved in computational studies in chemistry and biology, especially those who want a deeper understanding of the underlying representations of intra- and intermolecular energetics."

Prof. William L. Jorgensen
Yale University, USA

As computational hardware continues to develop at a rapid pace, quantitative computations are playing an increasingly essential role in the study of biomolecular systems. One of the most important challenges that the field faces is to develop the next generation of computational models that strike the proper balance of computational efficiency and accuracy, so that the problems of increasing complexity can be tackled in a systematic and physically robust manner. In particular, properly treating intermolecular interactions is fundamentally important for the reliability of all computational models. In this book, contributions by leading experts in the area of biomolecular simulations discuss cutting-edge ideas regarding effective strategies to describe many-body effects and electrostatics at quantum, classical, and coarse-grained levels. The goal of the book is to not only provide an up-to-date snapshot of the current simulation field but also stimulate exchange of ideas across different sub-fields of modern computational (bio) chemistry. The text will be a useful reference for the biomolecular simulation community and help attract talented young students into this exciting frontier of research.



Qiang Cui is professor of chemistry at the University of Wisconsin-Madison, USA. He is interested in developing theoretical/computational methods for the analysis of biomolecular systems, especially concerning chemical reactions in enzymes, energy transduction in biomolecular machines, and, more recently, interaction between biomolecules, lipids, and inorganic materials.



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