
Contents

Series Preface	xi
Preface	xiii
Editor	xv
Contributors	xvii

SECTION I Advanced Simulation Techniques

- 1 Introduction to Molecular Dynamics and Enhanced Sampling Algorithms 3
Xuhui Huang, Ruhong Zhou, and Bruce J. Berne
- 2 Toward Quantitative Analysis of Metalloenzyme Function Using MM and Hybrid QM/MM Methods: Challenges, Methods, and Recent Applications 33
Michael Gaus, Puja Goyal, Guanhua Hou, Xiya Lu, Xueqin Pang, Jan Zienau, Xin Xu, Marcus Elstner, and Qiang Cui
- 3 Development of AMOEBA Force Field with Advanced Electrostatics 83
Zhen Xia, Qiantao Wang, Xiaojia Mu, and Pengyu Ren

SECTION II Self-Assembly of Biomolecules

- | | | |
|---|---|-----|
| 4 | Molecular Simulations of Protein Folding Dynamics and Thermodynamics
<i>Deepak R. Canchi, Charles English, Camilo A. Jimenez-Cruz, and Angel E. Garcia</i> | 111 |
| 5 | Minimal Models for the Structure and Dynamics of Nucleic Acids
<i>Changbong Hyeon and Devarajan (Dave) Thirumalai</i> | 141 |
| 6 | Amyloid Peptide Aggregation: Computational Techniques to Deal with Multiple Time and Length Scales
<i>Luca Larini and Joan-Emma Shea</i> | 165 |
| 7 | Lipid Bilayers: Structure, Dynamics, and Interactions with Antimicrobial Peptides
<i>Yi Wang and J. Andrew McCammon</i> | 191 |

SECTION III Biomolecular Interactions

- | | | |
|----|--|-----|
| 8 | Protein and Nucleic Acid Interactions with Molecular Dynamics Simulations
<i>Zhen Xia and Ruhong Zhou</i> | 217 |
| 9 | Simulating Membranes and Membrane Proteins
<i>Nicholas Leioatts and Alan Grossfield</i> | 243 |
| 10 | Protein and Nanoparticle Interactions: Perspectives of Nanomedicine and Nanotoxicity
<i>Seung-gu Kang and Ruhong Zhou</i> | 277 |

SECTION IV More Applications in Molecular Biology

11 Modeling of DNA Sequencing with Solid-State Nanopores	311
<i>Binquan Luan</i>	
12 Biological Water under Confinement: Nanoscale Dewetting	329
<i>Ruhong Zhou</i>	
Index	353