1. Record Nr. UNINA9910298287503321

| | |
|---|---|
| Titolo | Computational Electrostatics for Biological Applications : Geometric and Numerical Approaches to the Description of Electrostatic Interaction Between Macromolecules / / edited by Walter Rocchia, Michela Spagnuolo |
| Pubbl/distr/stampa | Cham : , : Springer International Publishing : , : Imprint : Springer, , 2015 |
| ISBN | 3-319-12211-8 |
| Edizione | [1st ed. 2015.] |
| Descrizione fisica | 1 online resource (311 p.) |
| Disciplina | 006.6<br>516<br>530.1<br>570<br>570.285<br>570285<br>571.4 |
| Soggetti | Bioinformatics<br>Computational biology<br>Biophysics<br>Biological physics<br>Biomathematics<br>Mathematical physics<br>Computer graphics<br>Geometry<br>Computer Appl. in Life Sciences<br>Biological and Medical Physics, Biophysics<br>Mathematical and Computational Biology<br>Theoretical, Mathematical and Computational Physics<br>Computer Graphics |
| Lingua di pubblicazione | Inglese |
| Formato | Materiale a stampa |
| Livello bibliografico | Monografia |
| Note generali | Description based upon print version of record. |
| Nota di bibliografia | Includes bibliographical references. |

Nota di contenuto

Foreword; Preface; Contents; 1 Electrostatics Models for Biology; 1.1 Introduction; 1.2 Protein--Nucleic Acid Interactions; 1.3 Protein--Protein Interactions; 1.4 pH-Dependence and pKa Calculations; 1.5 Protein Solubility and Aggregation; 1.6 pH Variation and Subcellular Compartments; 1.7 Conclusion; References; 2 Classical Density Functional Theory of Ionic Solutions; 2.1 Introduction; 2.2 Classical DFT of Simple Fluids; 2.2.1 The Generalized van der Waals' Theory; 2.2.2 Grand Potential and Symmetry; 2.3 DFT of Simple Ionic Systems; 2.3.1 Poisson--Boltzmann DFT
2.3.2 Approximating Ion Correlations2.4 Examples; 2.4.1 Interaction Between Two Charged Colloidal Particles; 2.4.2 Adsorption of Polyions to Oppositely Charged Surfaces; 2.5 Conclusions; References; 3 A Comprehensive Exploration of Physical and Numerical Parameters in the Poisson--Boltzmann Equation for Applications to Receptor--Ligand Binding; 3.1 Introduction; 3.2 Methods and Materials; 3.3 Results and Discussion; 3.3.1 Physical Parameters and Features; 3.3.2 Numerical Parameters; 3.3.3 Experimental Validation; 3.4 Conclusion; References
4 The Adaptive Cartesian Grid-Based Poisson--Boltzmann Solver: Energy and Surface Electrostatic Properties4.1 Introduction; 4.1.1 Meshing Options; 4.1.2 The Adaptive Cartesian Grid-Based Poisson--Boltzmann Solver (CPB); 4.2 Methods; 4.2.1 Least Squares-based Reconstruction (LSR); 4.2.2 Comment on Surface Discontinuities; 4.3 Results; 4.3.1 Mesh Convergence Tests; 4.3.2 Energy-Based Poisson--Boltzmann Properties; 4.3.3 Electrostatic Solvation Free Energies of Biomolecules; 4.3.4 Electrostatic Binding Free Energies; 4.3.5 Surface-Based Electrostatic Properties; 4.3.6 Sphere Model Problem
4.3.7 Electrostatic Potential Mapped on Realistic Biomolecular Surfaces4.3.8 Net Induced Surface Charge and Forces for Realistic Biomolecular Geometries; 4.3.9 Poisson--Boltzmann Forces; 4.4 Conclusions; References; 5 Efficient and Stable Method to Solve Poisson--Boltzmann Equation with Steep Gradients; 5.1 Introduction; 5.2 Poisson--Boltzmann Equation; 5.3 Invertible Mappings for PBE; 5.4 Numerical Test; 5.5 Conclusion; References; 6 Boundary-Integral and Boundary-Element Methods for Biomolecular Electrostatics: Progress, Challenges, and Important Lessons from CEBA 2013; 6.1 Overview
6.2 Background6.3 Computational Workflow; 6.3.1 New Applications for Computational Geometry; 6.3.2 Emerging Workflow Challenges for Meshing; 6.4 New Applications for Boundary-Integral Formulations; 6.4.1 Enclosing Surfaces; 6.4.2 Multiple Biomolecules; 6.5 New Approaches to Discretization; 6.6 Collaborative Efforts to Validate Numerical Methods; 6.7 Discussion; References; 7 The Accuracy of Generalized Born Forces; 7.1 Introduction; 7.2 Electrostatic Forces in Inhomogeneous Continuous Media; 7.3 Generalized Born Models; 7.4 The Accuracy of Generalized Born Versus Poisson--Boltzmann Forces
7.4.1 GBR6 Surface Integral Approximation Model

Sommario/riassunto

This book presents established and new approaches to perform calculations of electrostatic interactions at the nanoscale, with particular focus on molecular biology applications. It is based on the proceedings of the Computational Electrostatics for Biological Applications international meeting, which brought together researchers in computational disciplines to discuss and explore diverse methods to improve electrostatic calculations. Fostering an interdisciplinary approach to the description of complex physical and biological problems, this book encompasses contributions originating in the fields of geometry processing, shape modeling, applied mathematics, and computational biology and chemistry. The main topics covered are theoretical and numerical aspects of the solution of the Poisson-

Boltzmann equation, surveys and comparison among geometric approaches to the modelling of molecular surfaces and related discretization and computational issues. It also includes a number of contributions addressing applications in biology, biophysics and nanotechnology. The book is primarily intended as a reference for researchers in the computational molecular biology and chemistry fields. As such, it also aims at becoming a key source of information for a wide range of scientists who need to know how modeling and computing at the molecular level may influence the design and interpretation of their experiments.