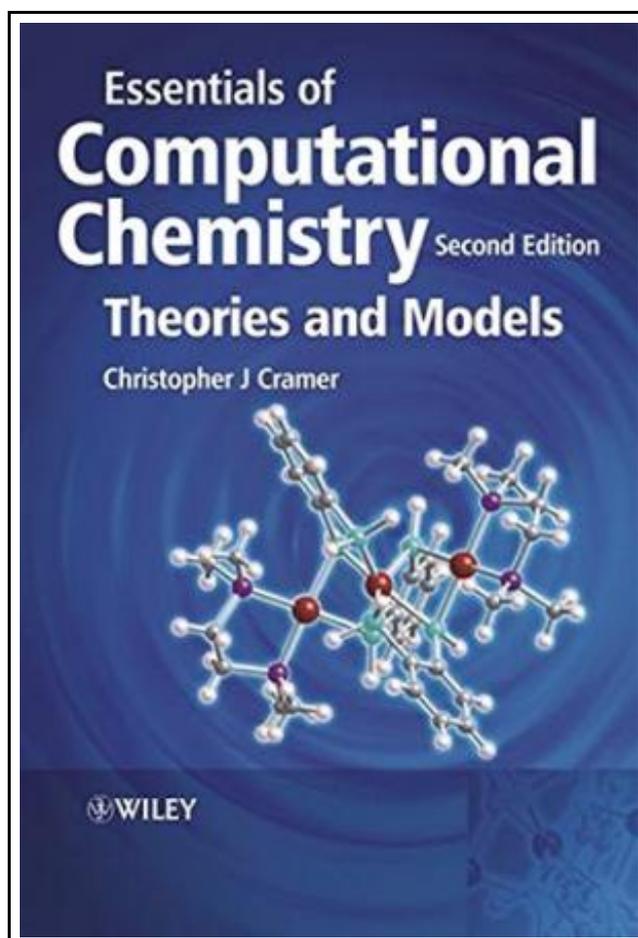


Essentials of Computational Chemistry: Theories and Models



Filesize: 6.79 MB

Reviews

Definitely among the best book I have possibly read. I have study and i am sure that i will going to go through once more once more later on. Your lifestyle span is going to be convert when you full looking at this publication.

(Prof. Damon Kautzer III)

ESSENTIALS OF COMPUTATIONAL CHEMISTRY: THEORIES AND MODELS



Wiley, 2004. Book Condition: New. Brand New, Unread Copy in Perfect Condition. A+ Customer Service!
Summary: Preface to the First Edition. Preface to the Second Edition. Acknowledgments. 1. What are Theory, Computation, and Modeling? 1.1 Definition of Terms. 1.2 Quantum Mechanics. 1.3 Computable Quantities. 1.3.1 Structure. 1.3.2 Potential Energy Surfaces. 1.3.3 Chemical Properties. 1.4 Cost and Efficiency. 1.4.1 Intrinsic Value. 1.4.2 Hardware and Software. 1.4.3 Algorithms. 1.5 Note on Units. Bibliography and Suggested Additional Reading. References. 2. Molecular Mechanics. 2.1 History and Fundamental Assumptions. 2.2 Potential Energy Functional Forms. 2.2.1 Bond Stretching. 2.2.2 Valence Angle Bending. 2.2.3 Torsions. 2.2.4 van der Waals Interactions. 2.2.5 Electrostatic Interactions. 2.2.6 Cross Terms and Additional Non-bonded Terms. 2.2.7 Parameterization Strategies. 2.3 Force-field Energies and Thermodynamics. 2.4 Geometry Optimization. 2.4.1 Optimization Algorithms. 2.4.2 Optimization Aspects Specific to Force Fields. 2.5 Menagerie of Modern Force Fields. 2.5.1 Available Force Fields. 2.5.2 Validation. 2.6 Force Fields and Docking. 2.7 Case Study: (2R*,4S*)-1-Hydroxy-2,4-dimethylhex-5-ene. Bibliography and Suggested Additional Reading. References. 3. Simulations of Molecular Ensembles. 3.1 Relationship Between MM Optima and Real Systems. 3.2 Phase Space and Trajectories. 3.2.1 Properties as Ensemble Averages. 3.2.2 Properties as Time Averages of Trajectories. 3.3 Molecular Dynamics. 3.3.1 Harmonic Oscillator Trajectories. 3.3.2 Non-analytical Systems. 3.3.3 Practical Issues in Propagation. 3.3.4 Stochastic Dynamics. 3.4 Monte Carlo. 3.4.1 Manipulation of Phase-space Integrals. 3.4.2 Metropolis Sampling. 3.5 Ensemble and Dynamical Property Examples. 3.6 Key Details in Formalism. 3.6.1 Cutoffs and Boundary Conditions. 3.6.2 Polarization. 3.6.3 Control of System Variables. 3.6.4 Simulation Convergence. 3.6.5 The Multiple Minima Problem. 3.7 Force Field Performance in Simulations. 3.8 Case Study: Silica Sodalite. Bibliography and Suggested Additional Reading. References. 4. Foundations of Molecular Orbital Theory. 4.1 Quantum Mechanics and the Wave Function. 4.2 The Hamiltonian Operator. 4.2.1 General Features. 4.2.2 The Variational Principle. 4.2.3 The Born-Oppenheimer Approximation. 4.3 Construction of Trial...



[Read Essentials of Computational Chemistry: Theories and Models Online](#)



[Download PDF Essentials of Computational Chemistry: Theories and Models](#)

See Also



Grandpa Spanielson's Chicken Pox Stories: Story #1: The Octopus (I Can Read Book 2)

HarperCollins, 2005. Book Condition: New. Brand New, Unread Copy in Perfect Condition. A+ Customer Service! Summary: Foreword by Raph Koster. Introduction. I. EXECUTIVE CONSIDERATIONS. 1. The Market. Do We Enter the Market? Basic Considerations. How...

[Save eBook »](#)



The Web Collection Revealed, Premium Edition: Adobe Dreamweaver CS6, Flash CS6, and Photoshop CS6 (Stay Current with Adobe Creative Cloud)

Cengage Learning, 2012. Book Condition: New. Brand New, Unread Copy in Perfect Condition. A+ Customer Service! Summary: You can now maximize and integrate the design and development power of Adobe Creative Suite 6 with WEB...

[Save eBook »](#)



Star Flights Bedtime Spaceship: Journey Through Space While Drifting Off to Sleep

CreateSpace Independent Publishing Platform, 2013. Book Condition: New. Brand New, Unread Copy in Perfect Condition. A+ Customer Service! Summary: "Star Flights Bedtime Spaceship" is a charming and fun story with the purpose to help children...

[Save eBook »](#)



Maisy's Christmas Tree

Candlewick, 2014. Book Condition: New. Brand New, Unread Copy in Perfect Condition. A+ Customer Service! Summary: The final scene of the gang caroling around the tree, complete with paper crowns from British Christmas crackers, is...

[Save eBook »](#)



Theoretical and practical issues preschool(Chinese Edition)

paperback. Book Condition: New. Ship out in 2 business day, And Fast shipping, Free Tracking number will be provided after the shipment.Paperback. Pub Date :2013-09-01 Language: Chinese Publisher:. Huazhong Normal University Press only genuine new...

[Save eBook »](#)