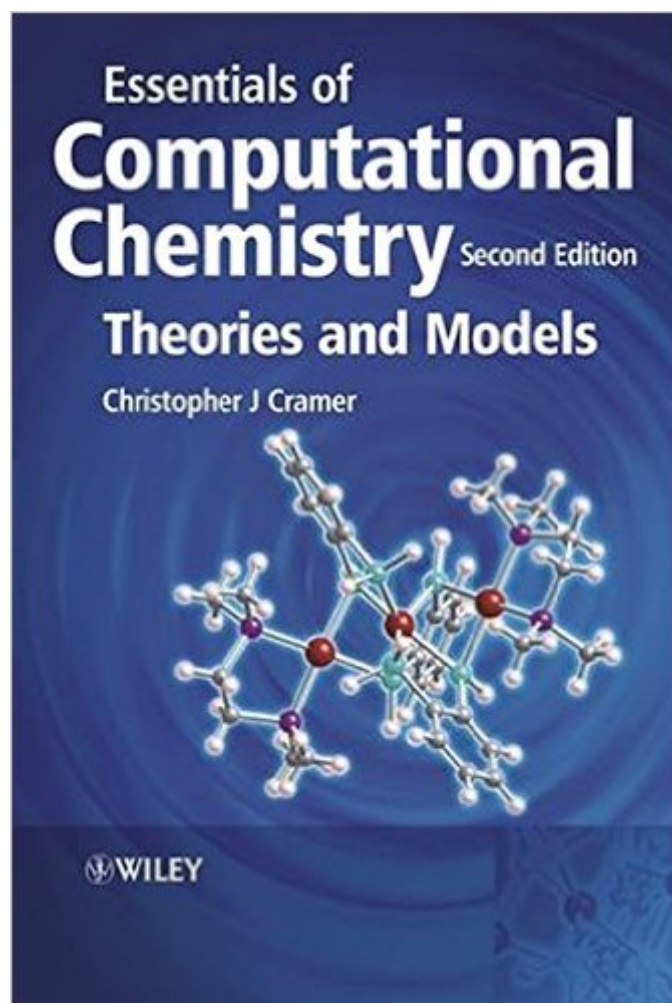# Essentials Of Computational Chemistry: Theories And Models

Synopsis

Essentials of Computational Chemistry provides a balanced introduction to this dynamic subject. Suitable for both experimentalists and theorists, a wide range of samples and applications are included drawn from all key areas. The book carefully leads the reader thorough the necessary equations providing information explanations and reasoning where necessary and firmly placing each equation in context.

Book Information

Paperback: 618 pages

Publisher: Wiley; 2 edition (October 29, 2004)

Language: English

ISBN-10: 0470091827

ISBN-13: 978-0470091821

Product Dimensions: 6.7 x 1.1 x 9.7 inches

Shipping Weight: 2.3 pounds (View shipping rates and policies)

Average Customer Review: 4.6 out of 5 stars See all reviews (16 customer reviews)

Best Sellers Rank: #108,452 in Books (See Top 100 in Books)   #41 in Books > Science & Math > Chemistry > Physical & Theoretical   #81 in Books > Medical Books > Medicine > Internal Medicine > Pathology > Clinical Chemistry   #349 in Books > Textbooks > Science & Mathematics > Chemistry

Customer Reviews

This book is a follow-up to a previous release and is a great textbook for learning how to simulate atoms, molecules, and fluid mixtures using a variety of techniques. Its positive attributes includes the following:1. The author makes it a point to explain the various phrases, acronyms, and terms common in the field, but which may confuse the novice or outsider. For example, the first chapter explains the concept of a potential energy surface, how it can be obtained, and the information that can be gleaned from it. These are simple concepts to those experienced in atomistic modeling but can be mysterious to newcomers.2. The mathematics in the text are simple enough to be understood without the reader having to resort to proving things herself, but they are complete enough to understand how physical concepts are represented and solved. The equations are also set apart from the text such that they are easy to read.3. There are a lot of diagrammatic figures that explain what is going on; i.e. how atoms interact via certain empirical potentials. One can also tell that the figures were made specifically to teach a concept, and are not reproductions from a

publication.4. The text is appropriate for first-year graduate students in physics, engineering, and chemistry, and the book provides chapters dedicated to quantum mechanics and thermodynamics, the two topics science and engineering students have the most difficulty in.5. The case study at the end of each chapter are well laid out and do a good job of illustrating the concepts taught in that chapter.6. There are a lot of flowcharts that show the process by which a calculation is carried out. See for example the appendix on determining the point symmetry of a molecule.

Essentials of Computational Chemistry: Theories and Models In Silico Medicinal Chemistry: Computational Methods to Support Drug Design (Theoretical and Computational Chemistry Series) Computational Photochemistry, Volume 16 (Theoretical and Computational Chemistry) Computational Fluid Mechanics and Heat Transfer, Third Edition (Series in Computational and Physical Processes in Mechanics and Thermal Sciences) Philosophies And Theories For Advanced Nursing Practice (Butts, Philosophies and Theories for Advanced Nursing Practice) Nursing Theories and Nursing Practice (Third Edition) (Parker, Nursing Theories and Nursing Practice) Complexity in Chemistry, Biology, and Ecology (Mathematical and Computational Chemistry) Theories for Direct Social Work Practice (SW 390N 2-Theories of Social Work Practice) Theories of Personality (PSY 235 Theories of Personality) Interdisciplinary Interaction Design: A Visual Guide to Basic Theories, Models and Ideas for Thinking and Designing for Interactive Web Design and Digital Device Experiences Digital Scholarly Editing: Theories, Models and Methods (Digital Research in the Arts and Humanities) Advances in Artificial Intelligence: Theories, Models, and Applications: 6th Hellenic Conference on AI, SETN 2010, Athens, Greece, May 4-7, 2010. Proceedings (Lecture Notes in Computer Science) Lenses on Reading, Second Edition: An Introduction to Theories and Models An Introduction to the Policy Process: Theories, Concepts, and Models of Public Policy Making Ace General Chemistry I and II (The EASY Guide to Ace General Chemistry I and II): General Chemistry Study Guide, General Chemistry Review Ace Organic Chemistry I: The EASY Guide to Ace Organic Chemistry I: (Organic Chemistry Study Guide, Organic Chemistry Review, Concepts, Reaction Mechanisms and Summaries) Ace General Chemistry I: The EASY Guide to Ace General Chemistry I: (General Chemistry Study Guide, General Chemistry Review) Microsoft Excel 2013 Building Data Models with PowerPivot: Building Data Models with PowerPivot (Business Skills) Modern Essentials Bundle - Modern Essentials *7th Edition* a Contemporary Guide to the Therapeutic Use of Essential Oils, an Intro to Modern Essentials, Reference Card, and Aroma Designs Bookmark Prepper Essentials: Prepper Essentials What Every Survivalist Needs To Know When Building The Ultimate SHTF Stockpile (Survival Handbook, DIY, Emergency ... Essentials

Books, Emergency Prepared)