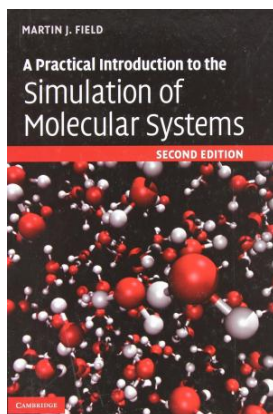


Read Book

A PRACTICAL INTRODUCTION TO THE SIMULATION OF MOLECULAR SYSTEMS



2015. Soft cover. Book Condition: New. 1st Edition. Preface to the first edition Preface to the second edition
 1 Preliminaries
 1.1 Introduction
 1.2 Python
 1.3 Object-oriented programming
 1.4 The pDynamo library
 1.5 Notation and units
 2 Chemical models and representations
 2.1 Introduction
 2.2 The System class
 2.3 Example 12
 2.4 Common molecular representations
 2.5 Example 23
 Coordinates and coordinate manipulations
 3.1 Introduction
 3.2 Connectivity
 3.3 Internal coordinates
 3.4 Example 33
 3.5 Miscellaneous transformations
 3.6 Superimposing structures
 3.7 Example 44
 Quantum chemical models
 4.1 Introduction
 4.2 The Born-Oppenheimer approximation
 4.3 Strategies for obtaining energies of a potential energy surface
 4.4 Molecular orbital methods
 4.5 The Hartree-Fock approximation
 4.6 Analysis of...

Read PDF A practical introduction to the simulation of molecular systems

- Authored by -
- Released at -



Filesize: 7.21 MB

Reviews

A superior quality publication and the font utilized was intriguing to read. I could comprehend every little thing using this composed e publication. You will like the way the author compose this publication.

-- **Mr. Demario Trantow**

I just began reading this pdf. It is actually written in straightforward words instead of hard to understand. Once you begin to read the book, it is extremely difficult to leave it before concluding.

-- **Jensen Bins**

Related Books

California Version of Who Am I in the Lives of Children? an Introduction to Early Childhood Education, Enhanced Pearson Etext with Loose-Leaf Version --

- **Access...**
- **History of the Town of Sutton Massachusetts from 1704 to 1876 (Paperback)**
- **Read Write Inc. Phonics: Blue Set 6 Storybook 6 the Jar of Oil (Paperback)**
- **The Right Kind of Pride: A Chronicle of Character, Caregiving and Community (Paperback)**
- **Billy & Buddy 3: Friends First**