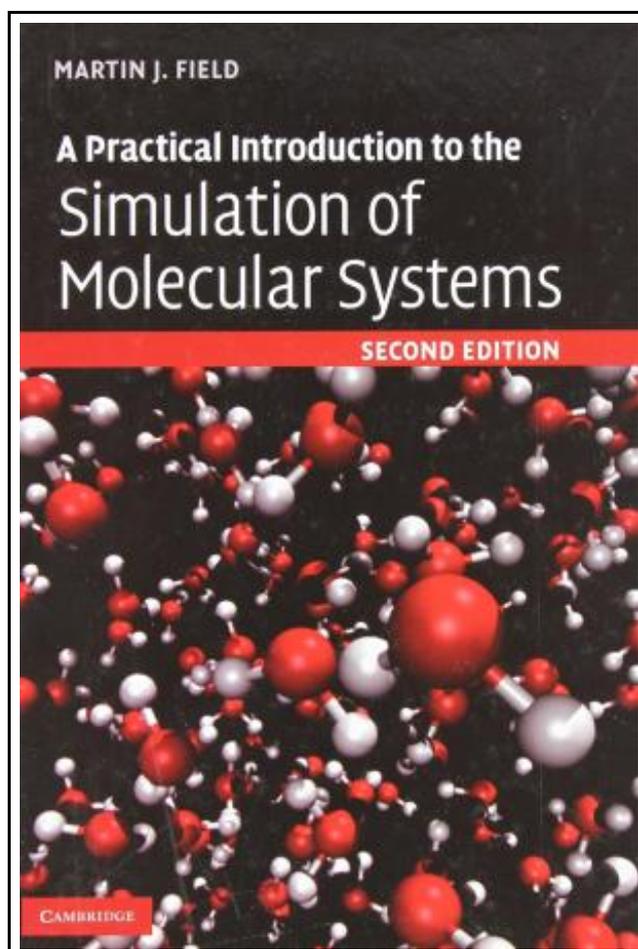


## A practical introduction to the simulation of molecular systems



Filesize: 6.75 MB

### ***Reviews***

*Undoubtedly, this is actually the best operate by any publisher. It is among the most amazing pdf i have got read. Its been printed in an exceptionally straightforward way which is just after i finished reading this book in which actually altered me, change the way i believe.  
(Deonte Kohler PhD)*

## 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  
 3 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  
 4 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 the charge density  
 4.7 Example 54  
 4.8 Derivatives of the potential energy  
 4.9 Example 65  
 5 Molecular mechanics  
 5.1 Introduction  
 5.2 Typical empirical energy functions  
 5.3 Calculating a molecular mechanics energy  
 5.4 Example 75  
 5.5 Parametrizing potential energy functions  
 5.6 Soft constraints  
 Hybrid potentials  
 6.1 Introduction  
 6.2 Combining QC and MM potentials  
 6.3 Example 86  
 6.4 Covalent bonds between QC and MM atoms  
 6.5 Example 9  
 Finding stationary points and reaction paths  
 of potential energy surfaces  
 7.1 Introduction  
 7.2 Exploring potential energy surfaces  
 7.3 Locating minima  
 7.4 Example 107  
 7.5 Locating saddle points  
 7.6 Example 117  
 7.7 Following reaction paths  
 7.8 Example 127  
 7.9 Determining complete reaction paths  
 7.10 Example 138  
 Normal mode analysis  
 8.1 Introduction  
 8.2 Calculation of the normal modes  
 8.3 Rotational and translational modes  
 8.4 Generating normal mode trajectories  
 8.5 Example 148  
 8.6 Calculation of thermodynamic quantities  
 8.7 Example 15  
 Appendix 1 The pDynamo library  
 Appendix 2 Mathematical appendix  
 Appendix 3 Solvent boxes and solvated molecules.



**[Read A practical introduction to the simulation of molecular systems Online](#)**  
**[Download PDF A practical introduction to the simulation of molecular systems](#)**

## Other 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 Card Package**

Pearson, United States, 2015. Loose-leaf. Book Condition: New. 10th. 249 x 201 mm. Language: English . Brand New Book. NOTE: Used books, rentals, and purchases made outside of Pearson If purchasing or renting from companies...

[Read PDF »](#)

---



**History of the Town of Sutton Massachusetts from 1704 to 1876 (Paperback)**

Createspace, United States, 2015. Paperback. Book Condition: New. annotated edition. 229 x 152 mm. Language: English . Brand New Book \*\*\*\*\* Print on Demand \*\*\*\*\*.This version of the History of the Town of Sutton Massachusetts...

[Read PDF »](#)

---



**Read Write Inc. Phonics: Blue Set 6 Storybook 6 the Jar of Oil (Paperback)**

Oxford University Press, United Kingdom, 2016. Paperback. Book Condition: New. Tim Archbold (illustrator). 148 x 148 mm. Language: N/A. Brand New Book. These engaging Storybooks provide structured practice for children learning to read the Read...

[Read PDF »](#)

---



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

Pearson, United States, 2015. Book. Book Condition: New. 10th. 250 x 189 mm. Language: English . Brand New Book. NOTE: Used books, rentals, and purchases made outside of Pearson If purchasing or renting from companies...

[Read PDF »](#)

---



**Who am I in the Lives of Children? An Introduction to Early Childhood Education (Paperback)**

Pearson Education (US), United States, 2015. Paperback. Book Condition: New. 10th Revised edition. 254 x 201 mm. Language: English . Brand New Book. Note: This is the bound book only and does not include access...

[Read PDF »](#)