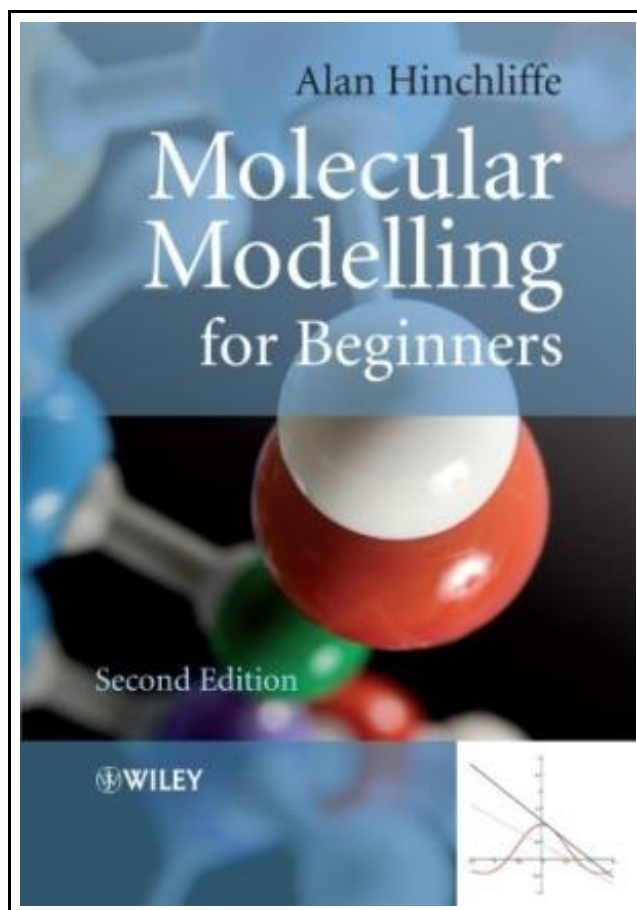


Molecular Modelling for Beginners



Filesize: 7.09 MB

Reviews

It is one of the best ebooks. Yes, it is actually engaging, still an interesting and amazing literature. It has been developed in an exceedingly straightforward way in fact it is just following it that I finished reading through this book by which basically modified me, altered the way I really believe.
(Mr. Maynard Kessler PhD)

MOLECULAR MODELLING FOR BEGINNERS

DOWNLOAD



Wiley, 2008. Book Condition: New. Brand New, Unread Copy in Perfect Condition. A+ Customer Service!
 Summary: Chapter 1: Electric charges and their properties.1.1 Point Charges.1.2 Coulomb's Law.1.3 Pair wise additivity.1.4 The Electric Field.1.5 Work.1.6 Charge distributions.1.7 The mutual potential energy U.1.8 Relationship between force and mutual potential energy.1.9 Electric Multipoles.1.10 The electrostatic potential.1.11 Polarization and Polarizability.1.12 Dipole polarizability.1.13 Many-body forces.1.14 Problem Set.Chapter 2: The Forces between Molecules.2.1 The Pair Potential.2.2 The multipole expansion.2.3 The Charge-Dipole interaction.2.4 The dipole-dipole interaction.2.5 Taking account of the temperature.2.6 The Induction energy.2.7 Dispersion energy.2.8 Repulsive contributions.2.9 Combination rules.2.10 Comparison with Experiment.2.11 Improved pair potentials.2.12 A Numerical potential.2.13 Site-site potentials.2.14 Problem Set.Chapter 3: Balls on Springs.3.1 Vibrational Motion.3.2 The Force Law.3.3 A simple diatomic.3.4 Three Problems.3.5 The Morse Potential.3.6 More Advanced Potentials.Chapter 4: Molecular Mechanics (MM).4.1 More about balls on springs.4.2 Larger systems of balls on springs.4.3 Force fields.4.4 Molecular Mechanics (MM).4.5 Modelling the solvent.4.6 Time-and-Money-saving tricks.4.7 Modern Force Fields.4.8 Some commercial force fields.Chapter 5: The Molecular Potential Energy Surface (PES).5.1 Multiple Minima.5.2 Saddle Points.5.3 Characterization.5.4 Finding Minima.5.5 Multivariate grid search.5.6 Derivative methods.5.7 First Order Methods.5.8 Second Order methods.5.9 Choice of Method.5.10 The Z matrix.5.11 The end of the Z matrix.5.12 Redundant Internal Coordinates.Chapter 6: Molecular Mechanics Examples.6.1 Geometry Optimization.6.2 Conformation Searches.6.3 Aminoacids.6.4 QSAR.6.5 Problem Set.Chapter 7: Sharing out the energy.7.1 Games of Chance.7.2 Enumeration.7.3 The Boltzmann Probability.7.4 Safety in Numbers.7.5 The Partition Function.7.6 A two-level quantum system.7.7 Lindemann's Theory of Melting.7.8 Problem Set.Chapter 8: Quick guide to Statistical Thermodynamics.8.1 The Ensemble.8.2 The Internal Energy Uth.8.3 The Helmholtz energy A.8.4 The entropy S.8.5 Equation of state and pressure.8.6 Phase space.8.7 The Configurational Integral.8.8 The Virial of Clausius.Chapter 9: Monte Carlo Simulations.9.1 Introduction.9.2 An Early Paper.9.3 The First "Chemical" Monte Carlo Simulation.9.4 Importance Sampling.9.5 The Periodic Box.9.6 Cutoffs.9.7 MC Simulation of Rigid Molecules.9.8 Flexible Molecules.Chapter 10: Molecular...



[Read Molecular Modelling for Beginners Online](#)



[Download PDF Molecular Modelling for Beginners](#)

Other eBooks



TJ new concept of the Preschool Quality Education Engineering the daily learning book of: new happy learning young children (2-4 years old) in small classes (3)(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 :2005-09-01 Publisher: Chinese children before making Reading: All books are the...

[Download eBook »](#)



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...

[Download eBook »](#)



Pickles To Pittsburgh: Cloudy with a Chance of Meatballs 2

Atheneum Books for Young Readers, 2000. Paperback. Book Condition: New. No Jacket. New paperback print book copy of Pickles to Pittsburgh: Cloudy with a Chance of Meatballs 2 written by Judi Barrett. Drawn by Ron...

[Download eBook »](#)



TJ new concept of the Preschool Quality Education Engineering the daily learning book of: new happy learning young children (3-5 years) Intermediate (3)(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 :2005-09-01 Publisher: Chinese children before making Reading: All books are the...

[Download eBook »](#)



Unplug Your Kids: A Parent's Guide to Raising Happy, Active and Well-Adjusted Children in the Digital Age

Adams Media Corporation. Paperback. Book Condition: new. BRAND NEW, Unplug Your Kids: A Parent's Guide to Raising Happy, Active and Well-Adjusted Children in the Digital Age, David Dutwin, TV. Web Surfing. IMing. Text Messaging. Video...

[Download eBook »](#)

**Read Write Inc. Phonics: Yellow Set 5 Non-Fiction 4 a Model Bird (Paperback)**

Oxford University Press, United Kingdom, 2016. Paperback. Book Condition: New. 197 x 116 mm. Language: N/A. Brand New Book. These decodable non-fiction books provide structured practice for children learning to read. Each set of books

[Read Document »](#)

**Read Write Inc. Phonics: Purple Set 2 Storybook 7 Flip Frog and the Bug (Paperback)**

Oxford University Press, United Kingdom, 2016. Paperback. Book Condition: New. Tim Archbold (illustrator). 162 x 136 mm. Language: N/A. Brand New Book. These engaging Storybooks provide structured practice for children learning to read the Read

[Read Document »](#)

**Read Write Inc. Phonics: Purple Set 2 Storybook 8 Red Ken (Paperback)**

Oxford University Press, United Kingdom, 2016. Paperback. Book Condition: New. Tim Archbold (illustrator). 253 x 147 mm. Language: N/A. Brand New Book. These engaging Storybooks provide structured practice for children learning to read the Read

[Read Document »](#)

**Read Write Inc. Phonics: Orange Set 4 Non-Fiction 3 Up in the Air (Paperback)**

Oxford University Press, United Kingdom, 2016. Paperback. Book Condition: New. 176 x 97 mm. Language: N/A. Brand New Book. These decodable non-fiction books provide structured practice for children learning to read. Each set of books

[Read Document »](#)

**Read Write Inc. Phonics: Purple Set 2 Storybook 6 Elvis (Paperback)**

Oxford University Press, United Kingdom, 2016. Paperback. Book Condition: New. Tim Archbold (illustrator). 196 x 148 mm. Language: N/A. Brand New Book. These engaging Storybooks provide structured practice for children learning to read the Read

[Read Document »](#)