



Molecular Modelling for Beginners

By Hinchliffe, Alan

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...



READ ONLINE
[2.31 MB]

Reviews

Most of these pdf is the greatest pdf available. It is really basic but excitement inside the fifty percent from the ebook. Your daily life span will likely be convert as soon as you complete reading this article ebook.

-- **Juwan Welch Sr.**

It in a of my personal favorite book. It really is filled with wisdom and knowledge Your daily life period will likely be enhance the instant you total looking at this pdf.

-- **Mr. Rocio Schroeder Sr.**

Other PDFs



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 Youth Pre-employment Training software download generated pictures...



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 Youth Pre-employment Training software download generated pictures...



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 Games. iPods. Kids today are plugged into...



RCadvisor s Modify: Design and Build From Scratch Your Own Modern Flying Model Airplane In One Day for Just

Rcadvisor.com, United States, 2009. Paperback. Book Condition: New. 238 x 166 mm. Language: English . Brand New Book ***** Print on Demand *****.Experience firsthand the joys of building and flying your very own model airplane design. Put into practice the lessons from...



Your Planet Needs You!: A Kid's Guide to Going Green

Macmillan Children's Books, 2009. Paperback. Book Condition: New. Rapidly dispatched worldwide from our clean, automated UK warehouse within 1-2 working days.



A Parent s Guide to STEM

U.S. News World Report, United States, 2015. Paperback. Book Condition: New. 214 x 149 mm. Language: English . Brand New Book ***** Print on Demand *****.This lively, colorful guidebook provides everything you need to know to help your child get inspired, succeed...