

Molecular modeling and polymer materials (with CD-ROM)(Chinese Edition)



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Reviews


Thorough information! Its such a good study. Sure, it is perform, still an amazing and interesting literature. Once you begin to read the book, it is extremely difficult to leave it before concluding.
(Evie Emmerich)

MOLECULAR MODELING AND POLYMER MATERIALS (WITH CD-ROM) (CHINESE EDITION)



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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: July. 2003 Pages: 336 in Publisher: Science Press molecular modeling and polymer materials introduced in recent years. the rapid development of new technologies that caught worldwide attention - molecular modeling the basic principles of molecular modeling in an effective way. as well as its applications in the research and design of polymer materials. Which is described by the computer from the atomic level to simulate the relationship of the macroscopic properties of polymer materials. prompted the chemical structure of the polymer materials and material. Molecular modeling software popular at home and abroad. such as MP and CERIUS2 of doing the introduction. Contents: Chapter molecule to simulate analog 1.3 Introduction 1.1 new field of 1.2 atomic level computer experimental the 1.4 test theories screening experiments 1.5 The third scientific research molecular field 2.1 vibrational spectra and force constants of 2.2 coordinates 2.3 spectrum force 4.1 The basic principle of the molecular dynamics method. Chapter 3.1 Basic principles of molecular mechanics methods. constant force field 2.4 experience potential function force field 2.5 charge balance method References Chapter 3.2 structure optimization direction 3.3 system pressure boundary 3.4 system References 4.2 numerical algorithm References Chapter 4.3 statistical sampling and macroscopic properties 4.4 statistical ensemble 4.5 system external force fields Reference Chapter molecular Monte Carlo method 5.1 real molecular Monte Carlo method 5.2 rotational isomeric state Monte Carlo method mesoscopic 7.5 Analysis of the scale the analog 6.1 mesoscopic scale computer simulation the 6.2 dynamic mean field density functional method 6.3 soft particle dynamics References Chapter VII of molecular modeling software (MP) 7.1 Overview 7.2 software features 7.3 file with the molecular structure of 7.4 calculated 9.1 Methods Chapter VIII of...

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