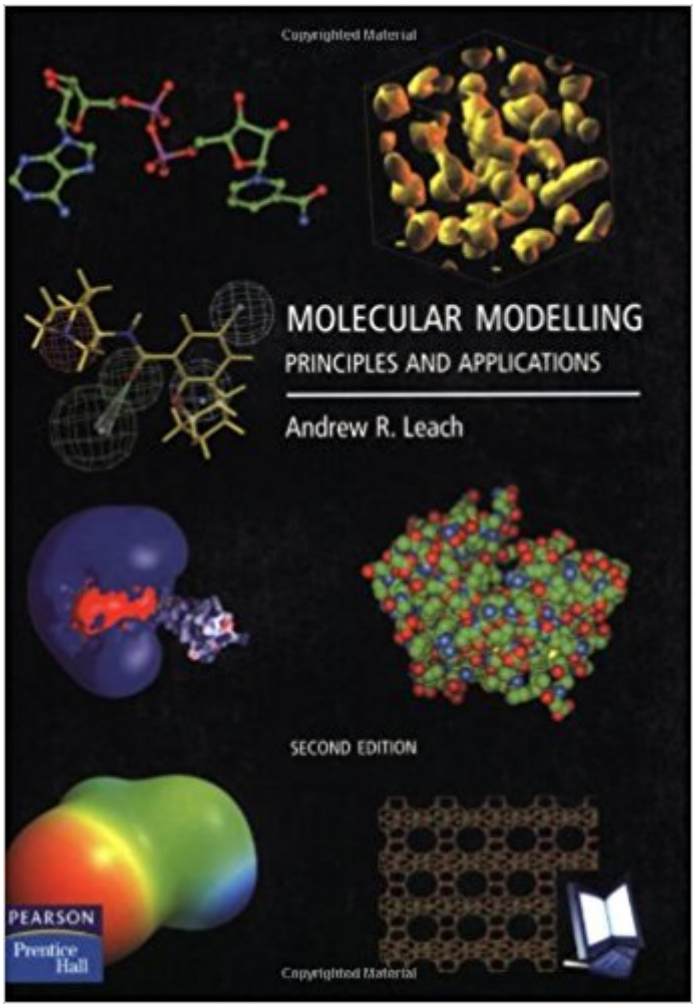
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Molecular Modelling: Principles And Applications (2nd Edition)



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Synopsis

This important new edition is for graduate students studying Molecular Modelling, Computational Chemistry within Chemistry,Ã Â Medicinal Chemistry and Biochemistry. Ã Â Postgraduates and researchers in academia and in the chemical and pharmaceutical industries. This new edition introduces background theory and techniques of molecular modelling, also illustrates applications in studying physical, chemical and biological phenomena.Ã Â It includes simple numerical examples and numerous explanatory figures and a colour plate section.Ã Â

Book Information

Paperback: 784 pages

Publisher: Pearson; 2 edition (April 9, 2001)

Language: English

ISBN-10: 0582382106

ISBN-13: 978-0582382107

Product Dimensions: 6.8 x 1.7 x 9.1 inches

Shipping Weight: 3.2 pounds (View shipping rates and policies)

Average Customer Review: 4.9 out of 5 stars 10 customer reviews

Best Sellers Rank: #114,711 in Books (See Top 100 in Books) #5 inÃ Â Books > Science & Math > Chemistry > Physical & Theoretical > Quantum Chemistry #22 inÃ Â Books > Science & Math > Chemistry > Molecular Chemistry #40 inÃ Â Books > Science & Math > Chemistry > Physical & Theoretical > Physical Chemistry

Customer Reviews

This important new edition is for postgraduate students of Chemistry, Medicinal Chemistry and Biochemistry studying Molecular Modelling and Computational Chemistry. The book will also be useful to researchers in academia and in the pharmaceutical and chemical industries and to those teaching or attending courses in molecular modelling. This new edition provides background theory in the techniques of molecular modelling, illustrated with applications form the physical, chemical and biological sciences. It includes simple numerical examples and numerous explanatory figures and a colour plate section. Key changes in this new edition * expanded coverage of materials science and solid-state modelling * extended chapter on drug design and chemoinformatics* new chapter on protein structure including bioinformatics* expanded coverage of Density Functional Theory Dr Andrew Leach is a Group Leader at Glaxo Wellcome Research and Development Limited and a Visiting Fellow at the Department of Chemistry, University of Southampton, UK

Dr. Andrew Leach is a Group Leader in Computational Chemistry and Informatics at Glaxo Wellcome Research and Development.

In this book, Andrew Leach has done a great job in describing almost every important concept, sundry as well as significant, from the field of computational chemistry and molecular modeling. From basic but very useful topics like atom types, Z matrices, and force field parametrization, to advanced ones like Ewald Sums and Low Mode Monte Carlo conformational searching, Leach gives due importance to everything. The discussions on quantum mechanics in the first few chapters are moderate on the mathematics without shying away from it, and provide just the right amount of detail. Later chapters cover the whole gamut of computational techniques, from molecular dynamics and molecular mechanics, to molecular similarity and QSAR. Examples that are relevant in chemistry and biology are scattered throughout the book and illustrate every key idea. There are many good books for computational chemistry and molecular modeling, and some are good for a few topics, others for other ones. However, if one wants to get a grip on all important topics in the area, I think this is the most comprehensive reference that one can look up.

EXCELLENT textbook for beginners in molecular and computational biophysics

A must have classic for simulation&theory people!

Good:This book gives an excellent overview of molecular simulation techniques starting with quantum mechanics ab initio type calculations and going up through molecular dynamics and polymer simulation. It gives a good step up from your standard physical chemistry text (such as Atkins or Chang) to being able to read the literature on modern molecular modelling techniques.Bad:The treatment of many methods is somewhat superficial.The book was first written in 1996 and updated in 2000 - it is starting to get a bit out of date.Overall I would recommend this as a solid introduction and reference.

This book is the gold standard survey of the fields of computational chemistry and molecular modeling. It is excellent for advanced undergraduates interested in the material, and also for graduate students working through rotations, course work, qualifying exams, and independent exploration. I also found it just plain interesting to read.When the book was recommended to me, a

colleague cautioned, "the only problem with the Leach book is how it communicates a superficial clarity--don't be mistaken in thinking you really understand the guts of the problem just because Leach communicates it so well." The advice was absolutely on point, and I think it serves to illustrate how well Leach has hit the target.

As we all know it's a great book on the subject, so there's nothing much to say about the book itself. The delivery was faster than expected and the book was in good shape. 5 stars !!!

Well, indeed it was a present and was not my idea.But my son, who's got the book, loves it ! Thanks.

I'd like to recommend this book from the perspective of someone who is new to the field. I have only an informal background in chemistry and biology and an undergraduate physics degree that's 20 years old. Mr. Leach works through a broad range of material, from numeric solutions to the quantum equations for a molecule to algorithms for searching through the conformational space. His descriptions have to be concise in order to fit the enormous volume of material he has to cover, yet I found that I had no trouble following along. He often takes a historical approach. I found this effective. I would find myself wandering down blind alleys when examining the early solutions, then read the later art and have a greater appreciation for the problem than if the ultimate answer were presented first. I have been able to use much of the book as a practical guide in my work.Frankly, I'm amazed that someone with a professional life can find the time to put together a book of this scope.

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