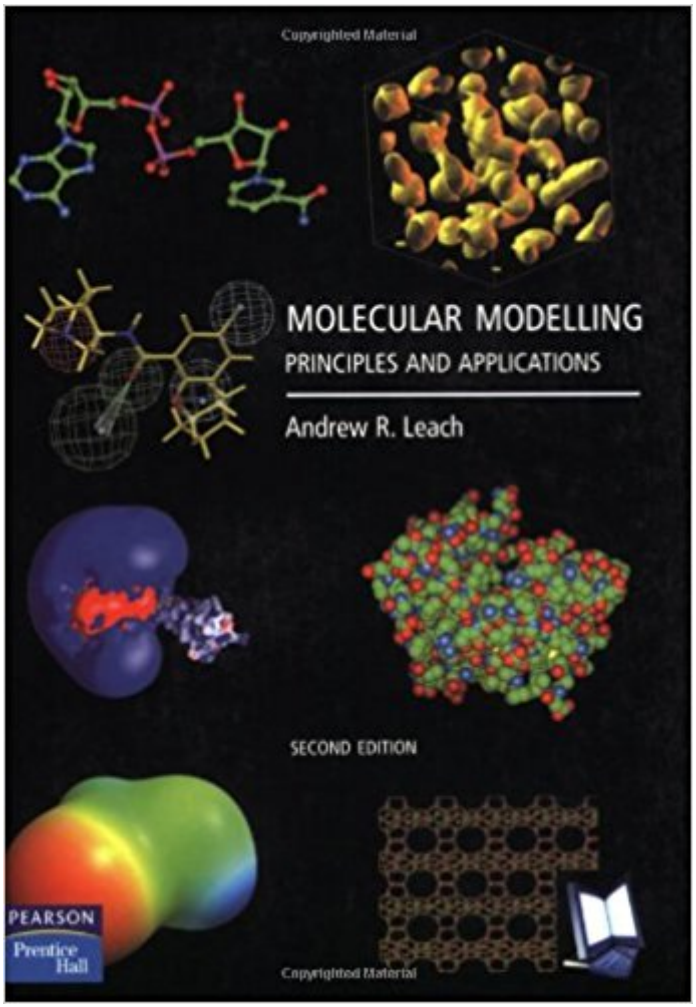
Molecular Modelling: Principles And Applications (2nd Edition)



Synopsis

This important new edition is for graduate students studying Molecular Modelling, Computational Chemistry within Chemistry,Â Medicinal Chemistry and Biochemistry. 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.Â It includes simple numerical examples and numerous explanatory figures and a colour plate section.Â

Book Information

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Customer Reviews

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.

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.

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.

If you could choose only one book about molecular modelling - this should be it. Everything is covered, more or less thourough, from ab initio to molecular docking, algorithms, force fields, molecular dynamics, etc. It is well written, but also works well if you want to look up single key words. The book can be read by novices to molecular modelling as well as it is useful for experts. I can highly recommend it.

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