Book Reviews

Molecular Modelling for Beginners. By Alan Hinchliffe. Wiley, Chichester, U.K. 2003. xviii + 410 pp. 17 × 24.5 cm. ISBN 0-4708-4310-1. $35.00.

This book does just what it says on the cover; it provides a comprehensive introduction to molecular modeling for beginners. Having said that, even though this is a book for beginners, the treatment is not simplistic and this is not an elementary text. As the author says in the preface, "many of the concepts and ideas are difficult ones, and you will have to think long and hard about them." There are elementary books on molecular modeling and there are classic and difficult texts, again as the author says in the preface, and the aim of this book is to take a middle course. It seems to me that this has been nicely achieved, and I was particularly pleased to see that all of the techniques used in modern molecular modeling have been put into proper historical context.

Following a brief introduction to chemical drawing, databases, file formats, and so on, there are three chapters that introduce the concepts necessary for an understanding of molecular mechanics, namely, electric charges, forces between molecules, and balls on springs. Molecular mechanics and force fields are covered in Chapter 5, followed by the molecular potential energy surface and a nice explanation of "minimization" methods, more accurately called optimization by the author. Chapter 7 gives a brief introduction to molecular mechanics calculations and conformational search and then discusses a small number of properties that may be computed in order to relate chemical structure to chemical or biochemical activity. This latter section is rather cursory and would perhaps have benefited from references to current reviews and books. Chapter 8 introduces statistical thermodynamics followed by a chapter on molecular dynamics and a chapter on Monte Carlo techniques. Quantum modeling appears in Chapter 11 and is then extensively discussed in the rest of the book, including density functional theory in Chapter 20. A chapter entitled "Miscellany" completes the text, followed by a useful mathematical appendix.

I was surprised to see that a book on molecular modeling did not include any color illustrations, although I suppose that this was a deliberate decision in order to keep the cost down. I would have liked to see a few more examples of classic modeling examples, which would make the book a bit more "hands on" for a beginner. This said, this is a well produced, well written book that I have no hesitation in recommending to a beginner in molecular modeling. Experienced users of molecular modeling packages may also find it useful, since it is possible to "drive" modeling software with little or no knowledge of the underlying theory.

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