Chemical Modeling: From Atoms to Liquids.
Alan Hinchliffe (Ed.), Wiley, 1999, 395 pp., £23.50 paperback, £55.00 hardback, ISBN 0-471-99903-2.

"Modeling means having a set of mathematical equations which are capable of representing accurately the phenomenon under study …" as phrased by Alan Hinchliffe in the introduction of his book *Chemical Modeling: From Atoms to Liquids*. Often one has to use a computer to turn such a set of equations into a tool to make predictions on the properties of molecules or materials. Computer simulation or molecular modelling is one of the most active and productive areas of research. The literature has grown exponentially in the past several years and great progress in both methodology and important applications has been reported. There clearly is a need to make undergraduate students aware of this development.

Whereas most chemical modelling books stop once the structure of one molecule has been discussed, Alan Hinchliffe continues and introduces statistical thermodynamics and modelling techniques to study the collective behaviour of molecules and atoms, which forms the basis of our understanding of the properties of materials. Chemical modelling is for many chemists a synonym for quantum chemistry calculations. The study of collective properties of molecules is often seen as the domain of physics, material science, or chemical engineering. Often this division can also be found in textbooks in these areas. The book of Hinchliffe is a refreshing exception.

The reader is given an introduction to thermodynamics, classical mechanics, quantum chemistry, statistical mechanics, Monte Carlo and molecular dynamics (MD) simulations, and polymer modelling. Although the subtitle is suggesting otherwise, theories on the solid phases are not ignored. The level at which the ideas and concept are introduced is appropriate for undergraduate students. The book successfully balances the need for mathematics and accessibility.

Writing a book with such a broad scope implies that the author has to cover a large spectrum of fields of active research. It is often a challenge to cover all topics with the same depth and insight. Clearly, Dr. Hinchliffe is an expert in the quantum chemical description of atoms and molecules. This expertise is reflected in a concise description of concepts and techniques to study the structure of atoms and molecules.

In the area of liquids the book is less successful. The role of computer simulations in the development of our current understanding of the structure of liquids is missing. At present, phase equilibria and thermodynamic properties of complex fluids can be predicted from Monte Carlo (MD) simulations. These are exciting developments of the last decade. It may be that these topics are too advanced for an undergraduate course. However, leaving the readers with the impression that one of the main applications of MD is to surpass barriers in a molecular mechanics calculation is, for someone who makes a living from this type of simulations, somewhat disappointing.

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