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BOOK REVEIW

Chemical Modeling, From Atoms to Liquids, by Alan Hinchliffe, 395 pages 179 figures, 78 tables, John Wiley & Sons., Chichester 1999, paperback. Price: 75.61 DM ISBN 0-471-99904-0 (hardcover 189.17 DM ISBN 0-471-99903-2)

The book gives a good review of aims, methods and results of chemical modeling. It consists of 21 chapters and eight appendices.

The *Introduction* explains notion, kind and methods of modeling, while chapter 1 *describes macroscopic systems* which will be modeled (6 pages, 1 figure, 2 tables).

The foundation – theoretical physics and computer simulation – of molecular modeling is described in 12 chapters: (2 *Thermodynamics* (15 pages, 2 figures, 4 tables); 3 *Résumé of classical mechanics* (21 pages, 11 figures); 5 *Introduction to quantum mechanics* (38 pages, 17 figures, 1 table); 6 *Electric multipoles, polarizabilities and intermolecular forces* (16 pages, 8 figures, 2 tables); 7 *Some statistical ideas* (23 pages, 10 figures, 20 tables); 8 *Application of the Boltzmann distribution* (12 pages, 8 figures); 10 *Molecular mechanics* (24 pages, 21 figures, 3 tables); 11 *Molecular dynamics and Monte Carlo techniques* (8 pages, 4 figures, 2 tables); 12 *The ideal monatomic gas* (5 pages, 1 figure); 13 *Quantum gases* (23 pages, 13 figures, 3 tables); 14 *Introduction to statistical thermodynamics* (20 pages, 2 figures, 2 tables); 19 *The band theory of solids* (14 pages, 9 figures, 2 tables).

These chapters give a clear and detailed description of the important analytical basis of chemical modeling; therefore, one can understand this basis without any additional reading.

Molecular mechanics, Molecular dynamics (MD) and Monte Carlo (MC) techniques establishing the basis for numerical calculations are also described in a good, understandable and concise manner. For a more detailed understanding of MD and MC one should consult additionally monographs of course (unfortunately not mentioned in the short *Suggestions for further reading*).

The remaining eight chapters [4 *Modeling simple solids (I)* (15 pages, 6 figures, 3 tables); 9 *Modeling simple solids (II)* (15 pages, 9 figures, 4 tables); 15 *Modeling atoms* (22 pages, 13 figures, 2 tables) 16 *Diatomics* (21 pages, 14 figures, 4 tables); 17 *Quantum modeling of larger systems* (34 pages, 9 figures, 14 tables); 18 *Describing electronic correlation* (14 pages, 7 tables); 19 *The band theory of solids* (14 pages, 9 figures, 2 tables); 20 *Modeling polymeric material* (11 pages, 5 figures, 1 table); 21 *Modeling liquids* (13 pages, 7 figures, 2 tables)] explain the main aim of the book *Chemical Modeling*.

In these chapters not only the principles of the modeling of different systems (including a short introduction to density functional theory) are given in a instructive manner but additionally a lot of examples to illustrate the procedure of the modeling.

Mathematical appendices, an index (very meager) and a short literature list complete the book.

This book is written clearly and understandably – although it seems in some sense very individually organized (e.g. the elements of statistical physics are distributed over five chapters) – and contains 179 excellent figures to improve the understanding of the complex material.

Thus the book is a valuable contribution to understanding the behavior of solids, liquids and gases in terms of the basic properties of their atoms, molecules and polymer chains as well as the inter- and intramolecular interaction between them.

Summarizing, it can be highly recommended not only for undergraduates but for graduates in chemistry, physical chemistry, material science and physics as well.

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