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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03 Chemical Kinetics and Inverse Modelling Problems. 04 Model Reduction Techniques for Chemical Mechanisms. 05 Vibrational and Chemical Kinetics in Non-Equilibrium Gas Flows. 06 Numerical Analysis of the Effect of Inhomogeneous Pre-Mixture on Pressure Rise Rate in HCCI Engine by Using Multi-Zone Chemical Kinetics.Â 13 Progresses in Experimental Study of N2 Plasma Diagnostics by Optical Emission Spectroscopy. 14 Nanoscale Liquid is Second Liquid. Part 5_ Application of Chemical Kinetics. 15 Application of Catalysts to Metal Microreactor Systems. Computational chemistry and process systems engineering play a major role in providing new understanding and development of computational procedures for the simulation, design, and operation of systems ranging from atoms and molecules to industrial-scale processes. The enormous span of scales of space and time that range from computational chemistry to process systems engineering can be visualized with the â€œchemical supply chainâ€ shown in Figure 6-1. Royal Society of Chemistry, 2010. 552 p. â€” ISBN 978-1-84973-035-8. There is increasing recognition that low-cost, high capacity processes for the conversion of biomass into fuels and chemicals are essential for expanding the utilization of carbon neutral processes, reducing dependency on fossil fuel resources, and increasing rural income. While much attention has focused on the use of biomass to produce ethanol via fermentation, high capacity processes are also required for the production of hydrocarbon fuels and chemicals from lignocellulosic biomass. schools in liquid-liquid extraction and inverse voltammetry.Â The second task discussed is the validation of the regression models with the aid of the cross-validation (CV) procedures. The leave-one-out (LOO) as well as the leave-many-out CV methods are used to evaluate the prognostic possibilities of QSAR. In the case of noisy and/or heterogeneous data the LM method is shown to exceed sufficiently the LS one with respect to the suitability of the regression models built.Â Thus to make modeling possible one should reduce the range of accounted chemical interactions that leads to simplification of chemico-physical model of process. The mathematical description of simplified model allows prediction of systemâ€™s behavior under different external actions. Chemical Modeling. From Atoms to Liquids. This edition was published in November 1, 1999 by Wiley. First Sentence. "Most chemical systems consist of very large numbers of atoms and molecules; a mole of any substance contains 6.022 x 1023 particles, a number of breathtaking and unimaginable magnitude." Classifications. Library of Congress. QD455.3.C64 H46 1999. ID Numbers. Open Library. OL7632413M.