Alan Hinchliffe
Chemical Modeling – From Atoms to Liquids

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This book was written by Alan Hinchliffe, Reader in Chemistry at the University of Manchester Institute of Science and Technology (Manchester, England, UK). The author's intention is to explain the procedures by which the properties of atoms, small and large molecules, solids, polymeric materials and liquids can be modeled. The present book is related to the author's earlier book *Modeling Molecular Structures* (John Wiley & Sons, Chichester, 1996).

Since modeling (that is, the process of model building) has been a philosophy of chemistry since its beginnings – even alchemists used models in their work, the author decided to present the mathematical and physical bases of modeling in chemistry. In the last decade or so the use of computers became especially useful for modeling in chemistry and science. Nowadays, it is wiser to construct first a model using a computer and then to test the model in real life. I remember Alan Hinchliffe from long ago, from our days at the University of Sheffield where we did graduate work under Professor (then young Lecturer) John N. Murrell FRS. Hinchliffe was already involved in modeling using computers (we worked on an old Feranti computer). Therefore, it is no wonder that in preparing this book he has used a computer and several sofware packages. These are briefly described and their Internet addresses are given at the beginning of the book under the title »*Software Packages*« (pp. XVII–XVIII).

The book consists of: Introduction (2 pages), Acknowledgments (1 page), Software Packages (2 pages), 21 chapters (370 pages), Appendix (18 pages; it gives the elements of mathematics used in the text), Suggestions for Further Reading (1 page) and Index (5 pages). Chapters are divided into those reporting introductory material and those dealing with applications. The book starts with the chapter »*Describing Macroscopic Systems*« (6 pages) in which the van der Waals, Beattie-Bridgeman, Benedict-Webb-Rubin and virial equations of the state and the principle of the corresponding states are given. The second chapter entitled »*Thermodynamics*« (15 pages) is a brief nonstandard introduction into classical thermodynamics. A very short section of the chapter is devoted to the Zeroth Law (see discussion about

this law in connection with the concept of zero in L. Pogliani, M. Randić and N. Trinajstić, *Much Ado About Nothing – An Introductory Inquiry About Zero*, *Int. J. Math. Educ. Sci. Technol.* **1998**, *29*, 729–744). The third chapter entitled »*Résumé of Classical Mechanics*« (21 pages) gives elements of classical mechanics. This chapter is followed by »*Modeling Simple Solids*« (First part) (15 pages) in which the author discusses the laws of electrostatics, the electrostatic field, the binding energy of a crystal, a simple ionic solid, *etc*. The fifth chapter (which is the longest chapter in the book) is again an introductory chapter entitled »*Introduction to Quantum Mechanics*« (38 pages) where the author presents the elements of the quantum mechanical approach to modeling the properties of microscopic systems (systems consisting of individual atoms and molecules). This as well as other introductory chapters are worth reading because the author in a succint manner informs the reader about the subject. The next chapter is entitled »*Electric Multipoles, Polarizabilities and Intermolecular Forces*« (16 pages), in which we learn about the intermolecular forces (forces between atoms in molecules), the electrostatic charge distribution, electrostatic potential, dielectric polarization, *etc*. The seventh chapter is entitled »*Some Statistical Ideas*« (23 pages). Tools of statistics are used when dealing with the properties of macroscopic systems (systems consisting of a very large number of atoms or molecules). Among the topics discussed are the Boltzmann distribution and the partition function. The next chapter entitled »*Applications of the Boltzmann Distribution*« (12 pages) is naturally linked to the previous chapter. The ninth chapter is entitled »*Modeling Simple Solids*« (Second part) (14 pages). Here the reader can learn something about materials engineering. We should remember that many man-made materials are much superior to natural materials. Thus, materials engineering (that is, preparing materials with desired properties) is one of the most important topics in science and technology research. The end of this chapter gives the answer to the question: »When do we need to use quantum mechanics?«

The tenth chapter entitled »*Molecular Mechanics*« (24 pages) is again an introductory chapter. In this chapter, the author describes computations using the molecular mechanics (MM) methodology and application of MM to study features of potential energy surfaces, protein docking, molecular properties, *etc*. The next chapter entitled »*Molecular Dynamics and Monte Carlo Techniques*« (8 pages) briefly describes how to solve the classical equations of motion for the atoms and molecules, given the intermolecular and intramolecular potentials, by means of molecular dynamics and the Monte Carlo method. In the twelfth chapter entitled »*The Ideal Monatomic Gas*« (5 pages), the author gives the classical and quantum derivation of an equation of state for an ideal monatomic gas. The thirteenth chapter entitled »*Quantum Gas*« (23 pages) contains, among other topics, the modeling of metals (for example, the mechanism of electrical conduction using the Drude electron gas model; later in the text the author returns to the Drude

model when discussing the band theory of solids, p. 332). The next chapter entitled »*Introduction to Statistical Thermodynamics*« (20 pages) is again a very useful introductory chapter. All the remaining chapters in the book are devoted to modeling.

The fifteenth chapter entitled »*Modeling Atoms*« (22 pages) discusses models of atoms from Bohr's model to the Hartree-Fock model, the Pauli principle and the Periodic Table. The next chapter entitled »*Diatomics*« (21 pages) presents the LCAO MO model of diatomic molecules. The seventeenth chapter is entitled »*Quantum Modeling of Larger Systems*« (34 pages) and discusses the HF-LCAO theory, Gaussian orbitals, Koopmans' theorem (Tjalling Charles Koopmans (1910–1985) shared the 1975 Nobel prize for economics with Leonid Vitaljevič Kantorovič (1912–1986)), geometry optimization, Hückel π-electron model, PPP models, all-valence electron ZDO models, *etc*. The next chapter entitled »*Describing Electron Correlation*« (14 pages) describes the configuration interaction, perturbation theory, Møller-Plesset perturbation procedure, density functional theory (Walter Kohn, who introduced density functional theory, shared the 1998 Nobel prize for chemistry with John A. Pople, who got it for his development of computational methods in quantum chemistry), *etc*. The nineteenth chapter entitled »*The Band Theory of Solids*« (14 pages) describes Drude's model of a metal, Ohms' law, Pauli's free electron model, the band theory, the Kronig-Penney model, semiconductors, *etc*. The next chapter entitled »*Modeling Polymeric Materials*« (12 pages) gives some ideas about modeling the properties of polymers. Finally, the twenty-first chapter entitled »*Modeling Liquids*« (13 pages) informs the reader about the internal energy of a liquid, classical and quantum liquids, describes the computer simulation of liquids, *etc*.

This book was written by a mature scientist whose aim was to teach the reader how to account for the behavior of gases, liquids and solids in terms of the properties of their atoms, molecules and polymer units. The author has succeeded admirably in his intention. I recommend this book to every chemist interested in the state-of-art chemical modeling techniques.

Nenad Trinajstić