Understanding Molecular Simulation: From Algorithms to Applications

Daan Frenkel, Berend Smit
(Academic Press, San Diego and London, 1996)
xviii+443 pages, $65.00
ISBN 0-12-267370-0

The realization of a parallel world of "digital definition" of new materials for particular applications may yet be some way in the future. In the meantime, simulations have gained their firm place in the array of techniques brought to bear on the task of understanding and developing materials. Molecular simulation, in particular, has grown into a mature technique not only in the life sciences, where its origins lie, but also in materials science. It is now easily accessible via a number of commercial software packages. As many have experienced, however, the initial joy of manipulating molecules on a computer screen can soon be replaced by frustration about not getting useful results.

The textbook by Frenkel and Smit hence offers hope to those struggling with the subject. Indeed it manages to deliver in many aspects. It provides an authoritative guide into and through the field, concentrating on phase equilibria "of molecular and supra-molecular substances." Starting from its foundations in statistical mechanics it goes on to deliver a detailed insight into the Monte Carlo and molecular dynamics methods with their many variations and tricks of the trade including advanced variants such as variable time-step, Gibbs ensemble and hybrid Monte Carlo techniques. The methods are outlined clearly and distinctly in the main text, supported by an extensive appendix (about 1/4 of the book). As befits a book on simulation, theory is illustrated by computer code. Little pseudo-code programs are found in the book itself, while full FORTRAN codes for a number of case studies discussed in the text can be downloaded from a website (http://molsim.chem.uva.nl/frenkel_smit). The site turns out to be much more than an archive, however. The authors have very recently added further material as well as case studies and codes which extend the scope of the book to areas such as parallel molecular dynamics simulations. It also provides a list of errata of which there are, unfortunately, quite a few, and not all of them trivial ones.

The book focuses on the generic behavior of the atomistic and molecular level. It does not, for example, cover aspects related to quantum mechanical effects, nor the Carr-Parrinello method which combines molecular dynamics with electronic structure calculations. Chemical detail, and issues for example concerning choice and validity of parameters for intermolecular potentials, are beyond its scope. However, there are other books covering that area, for example, *Molecular Modeling at the PC* by M.F. Schlecht (Wiley, New York, 1998).

In sum, even if one book cannot solve all of the problems, *Understanding Molecular Simulation* manages to address a great many of them. I strongly recommend it to anybody involved in the study, development, or application of molecular simulation.

Reviewer: *Gerhard Goldbeck-Wood received a doctorate at Aachen in polymer physics (1992), in the field of simulation of polymer crystallization. He pursued this topic, by both simulation and experiment, at Bristol, then worked for Molecular Simulations Inc., before joining the polymer group in the Department of Materials Science at Cambridge University; there he works on polymeric liquid crystals, both modeling and experiment, at all scales from the molecular to the macroscopic.*

Modern Thermodynamics: From Heat Engines to Dissipative Structures

Dilip Kondepudi and Ilya Prigogine
(John Wiley & Sons, West Sussex, England, 1998)
xxi + 486 pages, $79.95
ISBN: 0-471-97393-9

The book *Modern Thermodynamics*, by D. Kondepudi and I. Prigogine, is unique in its presentation and coverage. Many of the subjects treated herein are omitted in many textbooks on thermodynamics and should be of high current interest since many of the processes that we deal with occur under conditions far-from-equilibrium.

The authors' stated purpose is to give an introduction to present-day thermodynamics, starting with its historical roots and proceeding to the thermodynamics description of far-from-equilibrium systems. The book is divided into five parts: Historical Roots: From Heat Engines to Cosmology; Equilibirum Thermodynamics; Fluctuations and Stability; Linear Nonequilibrium Thermodynamics; and Order Through Fluctuations. The first two sections are intended for a one-semester introductory undergraduate course and the last three for advanced undergraduate or graduate course.

The material of the first two sections is presented in the historical and almost chronological manner in which the basic principles of thermodynamics were developed. This method has certain appeal, but the average undergraduate students being exposed to the subject for the first time may find it disjointed, and difficult to obtain a coherent view of a given topic. The book is directed at students in chemistry, physics, and engineering; however, one has no difficulty in deciding that the authors are chemists.

The authors are to be applauded, however, for the matter included in the last three sections. A treatment of nonequilibrium systems is rarely included in such detail in textbooks. The omission of nonequilibrium situations in the standard texts often leave students with the feeling that the concepts of equilibrium thermodynamics can be directly applied to systems that are far-from-equilibrium.

Researchers in the areas of systems far-from-equilibrium and self-organized systems will find a wealth of information and insights from careful study of the material presented by Kondepudi and Prigogine. One might obtain these concepts from the literature but only those with a deep interest in thermodynamics will do so. This volume presents the information in a coherent and logical manner and is highly recommended to the research community.

Reviewer: *Carl J. McHargue is director of the Center for Materials Processing and professor of materials and engineering at the University of Tennessee—Knoxville. He has long been interested in the analysis of ion-solid interactions and the results of ion implantation and ion beam mixing in ceramic systems.*

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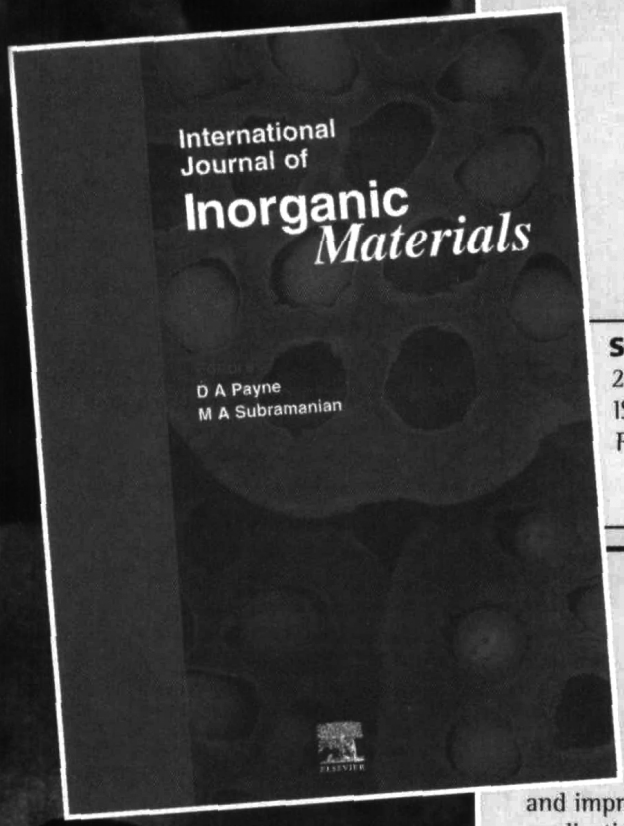

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