Molecular Crystals and Liquid Crystals Science and Technology. Section A. Molecular Crystals and Liquid Crystals

Publication details, including instructions for authors and subscription information:
http://www.tandfonline.com/loi/gmcl19

Book Reviews

Version of record first published: 04 Oct 2006

To cite this article: (1997): Book Reviews, Molecular Crystals and Liquid Crystals Science and Technology. Section A. Molecular Crystals and Liquid Crystals, 293:1, 325-331

To link to this article: http://dx.doi.org/10.1080/10587259708042780

Mol. Cryst. Liq. Cryst., 1997, Vol. 293, pp. 325–331
Reprints available directly from the publisher
Photocopying permitted by license only

*Book Reviews**

"An Introduction to Molecular Electronics", edited by Michael C. Petty, Martin R. Bryce, and David Bloor, Oxford University Press, New York, 1995; ISBN: 0-19-521156-1; xiv + 387 pages; $42.50.

This book was developed from a series of short courses given at the University of Durham during the summers of 1987–1991. Many of the chapters are contributed by the original lectures. The book is an attempt to bridge the boundaries of traditional disciplines, and it is aimed at final year undergraduates and research students from diverse backgrounds. The topics covered in this book have considerable overlap with those found in 'Molecular Electronics', edited by G. J. Ashwell, John Wiley & Sons, 1992, although there is considerably more coverage of biological topics in the present volume. This book deals with both the use of molecular materials for electronic, optical, and magnetic applications as well as electronic phenomena in molecular scale devices.

Following an overview chapter by D. Bloor and one on theory by R. W. Munn, the remaining 14 chapters deal with physical phenomena and molecular materials that exhibit them (e.g., conductive polymers), classes of materials and the phenomena they exhibit (e.g., liquid crystals), experimental techniques (e.g., scanning tunneling microscopy), potential applications (e.g., biosensors), and a futuristic essay ("Molecular Electronic Logic and Architectures").

In Chapter 8, "Conductive Charge-transfer Complexes", the statement that 'the first *stable* highly-conducting organic solids were reported by workers at DuPont laboratories in 1962" is inaccurate. The DuPont work on conductive TCNQ salts was reported earlier: D. S. Acker, *et al.*, *J. Am. Chem. Soc.*, **82**, 6408 (1960).

In Chapter 4, "Molecular Magnets", the authors correctly express reservations about the quality of the characterization of some of the materials claimed to be bulk ferromagnets. Their characterization of some of the claims as "irreproducible or even false" should probably have simply been termed irreproducible. They correctly call for substantiation of claims of

*Unsigned book reviews are by the Book Review Editor.

materials reported to be bulk ferromagnets. In that spirit, the Book Review Editor and his collaborators (M. Levinson, P. G. Rossoni, and E. A. Yost, unpublished experiments, 1991) reproduced the claim of ref. 23 of Chapter 4 of bulk ferromagnetism in polyaryl resins. However, the weight percentage of carbon and hydrogen in these amorphous materials decreased as a function of time.

In spite of the reservations noted above, students and individuals seeking initial information about the topics covered will find the chapters in this book quite readable and generally useful.

"Fundamental Principles of Molecular Modeling", edited by Werner Gans, Anton Amann, and Jan C. A. Boeyens, Plenum Press, New York, 1996; ISBN 0-306-45305-3; $79.50.

"Fundamental Principles of Molecular Modeling" edited by Werner Gans, Anton Amann and Jan C. A. Boeyens is the proceedings of an "indaba", that is a conference whose intent is to look at a difficult problem from all angles. This book does, indeed, look at the modeling of molecular systems from a wide variety of angles. This includes but is not limited to fundamental principles of quantum mechanics, detailed fitting of various experimental data, ab initio and semi-empirical calculations of electronic structure, discussions of the effect of the quantum delocalization of hydrogen bonding, molecular force-field based calculations of molecular and crystal structures etc.

Unfortunately for a scientist primarily interested in liquid crystals this range of topics does not include (except in a glancing way) thermal effects; force-field based finite temperature Monte-Carlo (for example) is entirely missing from the set of topics studied. The book will certainly be more useful for scientists interested in molecular crystals.

It was hard for this reviewer (and I expect for most single readers) to read the book with pleasure. Most chapters seem to be reasonably typical, good, well-written research papers in one or another of the diverse aspects of molecular modeling discussed at this conference. There is a great breadth of topics and almost all chapters discuss detailed state-of-the-art research in specific subtopics of each of these broad topics, all of which are interesting to certain practitioners of molecular modeling. Only a few have adequate introductory material to allow a well educated scientist to appreciate the discussion unless (s)he is already conversant with the broad topic discussed in that chapter. Some of the chapters deal with fundamentals, some with very practical problems and approaches to them. In consequence this book seems somewhat misnamed.

Reading the book gives a broad, if somewhat spotty, overview of what is currently possible in molecular modeling. It could be useful to scientists interested in such an overview.

Rolfe G. Petschek
Department of Physics
Case Western Reserve University
Cleveland, Ohio 44106-7079

"The Crystal as a Supramolecular Entity," edited by Gautam R. Desiraju, John Wiley & Sons, Chichester, West Sussex BP019 1UD, England, 1996; ISBN 0 471 950157; xi + 314 pages.

The study of materials in the crystalline state has become of increasing interest as the result of the highly interdisciplinary nature of the field and its wide range of applications in the chemical, engineering, physical and biological sciences. The progress in this discipline stems from the development of innovative methods for controlling molecular orientations in crystals and the evolution of computational resources available to researchers. New approaches towards the systematic design of crystalline materials, crystal engineering, have been successful in the prediction of rudimentary patterns in molecular crystals. The intent of this book is to clarify the perception of crystals as supramolecular entities by presenting current research developments in the area. As outlined by the editor and contributors, the terminology "supramolecular entity" encompasses materials that consist of long-range molecular periodicity, the product of directionally specific short-range interactions. Thus, crystals, not surprisingly, are considered supramolecular compounds. The selections presented in this book illustrate the diversity and scope of structural supramolecular chemistry.

Inspection of the manuscript reveals a diverse selection of authors and topics in the area of crystal engineering. The book consists of 314 pages containing recent references. Even though this is a multi-authored book, the entire text has a reasonable level of consistency and readability.

Chapter 1 (Dunitz) contains eloquent discussions on crystals as supermolecules with insights into the analyses of packing patterns of molecular crystals. This chapter builds upon the fundamental topics of polymorphism and crystal packing and concludes with discussions on the significance of quantifying crystal structures with molecular mechanics calculations. The main thrust of Chapter 2 (Desiraju and Sharma) focuses on molecular recognition and guest-host complexes. The analyses of several structural examples in the text provide insight into the self-assembly of molecular crystals. Chapter 3 (Davis, Whitesell, Wong and Chang) outlines an unique avenue towards crystal engineering by implementing molecular shape as the design tool. Unlike the traditional use of hydrogen bonds in structure prediction, this work emphasizes the use of molecular shape as the major determinant for crystal packing. Chapters 4 and 5 (Fagan and Ward, Dance, respectively) detail the

advances in crystal engineering in the lesser represented areas of oranometallic and inorganic materials. Each of these chapters cites specific structural examples and describes challenges unique to these disciplines. Appropriately, Chapter 6 (Glusker) concludes the book with discussions on predictions of the structure of life; crystal engineering in biomolecules. This work focuses on the determinant factors responsible for the architecture of $(\beta\alpha)_8$ barrel structural motifs in proteins.

Collectively these articles should be of interest to diverse groups in the areas of materials science and structural chemistry. Perceptions of these varying research topics have traditionally been segregated. The strength of this book is its ability to unite these disciplines by the common topical thread of supramolecular chemistry. As with all books of this type, the contents are not intended to be a comprehensive coverage of the discipline, but rather to provoke further discussion and future work.

Kraig A. Wheeler
Department of Chemistry
Delaware State University
Dover, DE 19901

Introduction to Solid State Physics; 7th Edition by Charles Kittel, John Wiley & Sons, Inc., New York, 1996; ISBN 0-471/-11181-3; $79.95.

This textbook is ideally suited for its intended audience of seniors and first year graduate students because it introduces the readers to the basic properties of solids and the fundamental concepts used to understand them in the first eight chapters. These chapters cover crystal structure, the reciprocal lattice, crystal bonding and elasticity, phonons, the free electron gas, energy bands and semiconductors. The background necessary to understand the material includes undergraduate quantum mechanics, thermodynamics and statistical physics. The variety of topics included allows this text to be used for a second course in which the basic concepts are applied to the properties of specific classes of materials such as dielectrics and magnetic materials and is extended to include excitations and deviations from perfect crystallinity.

The material is presented clearly and at a level appropriate to its audience incorporating the major experimental results and the models, both semiclassical and quantum mechanical, which explain them. However, no attempt is made to tie the models used to the fundamental quantum theory of solids at least qualitatively. This leaves the reader with the impression that solid state theory is nothing but a collection of disconnected mathematical models which happen to work for a particular ex-

periment. Although the many-body quantum theory of solids is certainly beyond the level of the students for whom this book was intended, at least its existence and a brief indication of the assumptions which reduce the general theory to the model being used would give the text a certain amount of continuity.

This latest edition of Charles Kittel's classic solid state physics textbook has been updated to include a variety of topics of current interest. New material has been added on high temperature superconductors and the Fullerences to the Superconductivity chapter. A section on nanostructures has been added to Chapter 6 on the Free Electron Fermi Gas, and a discussion of superlattices, Bloch/Wannier levels and Zener tunneling has replaced the topic of special crystals in the chapter on Semiconductor Crystals. Light emitting diodes and scanning tunneling microscopy have been added to the Surface and Interface Physics chapter, and an expanded discussion of fiber optic material has replaced the treatment of EXAFS in the chapter on Noncrystalline Solids. In addition, the topic of elastic constants and elastic waves which was dropped after the 4th edition has been restored to the chapter on Crystal Binding along with seven problems covering this area. Finally, a brief treatment of the hardness of materials has been included at the end of the chapter on Dislocations.

The problems at the end of the chapters are challenging and are intended to supplement the material in the text. However, the number of problems varies from ten or more problems in Chapters 3, 6, 9, 10 and 13 to five or less problems in Chapters 1, 5, 8, 17, 18, 19, 20 and 21. Unfortunately, the limited number of problems in some of the chapters coupled with the lack of variation in the level of difficulty of the problems does not give the student an opportunity to develop a thorough understanding of the material. Some lower level problems which are straightforward applications of the theory developed in the chapter, even if they are simple numerical calculations, would give the student a feel for the order of magnitude of the properties of solids.

In summary, I have used this textbook for a number of years and find it to be a good treatment of the phenomena of solid state physics at the introductory level. The minor shortcomings which I have mentioned above are not so serious that they cannot be remedied by supplementary material provided by the instructor.

A. S. Karakashian
Department of Physics and Applied Physics
University of Massachusetts Lowell
Lowell, Massachusetts 01854-2881

The Art of Molecular Dynamics Simulation. By Dennis C. Rapaport (Bar-Ilan University). Cambridge University Press: Cambridge, England. 1995. xiv + 400 pp. $69.95. ISBN 0-521-44561-2

It is difficult to imagine a book more informed and informative on the subject of classical molecular dynamics (MD) than this superb work. For the beginner as well as for the virtuoso in MD, this fascinating book will likely become required reading and a standard reference guide on the subject. At the same time, it should and will attract interest from anyone involved in computational chemistry in the broadest sense.

Described by the author as a "cookbook", it was written to be read either cover-to-cover as an introductory text on MD or selectively as a source of recipes for practical applications and physical properties of interest. The contents are organized into Chapters 1–15 plus Appendices A1–A6. Chapter 1 starts with some historical background on computer simulations, then compares MD with Monte Carlo (MC) and other dynamics methods employed as simulation tools. It concludes by summarizing the wide range of applications of MD, including: diffusion, phase transitions and critical phenomena, spectroscopic measurements, dielectric properties, mechanical properties, friction, and numerous other structural and dynamical properties of liquids, liquid crystals, polymers, membranes, and biomolecules, to name only a few. Chapter 2 introduces the basics of MD simulations (potential functions, periodic boundary conditions, integration algorithms, etc.) via the simple example of the Lennard-Jones (LJ) fluid. The reader is then treated to a feature that continues throughout the book: computer code (written in simplified C) to implement aspects of MD learned in that chapter. Throughout the book, the code is accompanied by an extensive discussion of computational details that any programmer or MD advocate, new and experienced, will find extremely useful. The author also graciously provides a World Wide Web site address at Cambridge University Press for downloading (apparently free of charge) the software described in the book. Chapter 3 discusses the methods and algorithms for simulating monatomic species with particular attention to paradigms for computing the atom-pair interactions (i.e., all pairs, cell subdivision, neighbor-list method) and to integration methods (e.g., leap-frog, predictor-corrector). Chapter 4 focuses on measuring the thermodynamic and structural properties of systems in equilibrium including those that can be verified experimentally (e.g., CV, radial distribution function). It also includes a welcomed section on constructing and analyzing Voronoi polyhedra. Chapter 5 covers the dynamical properties of equilibrium systems including transport coefficients (i.e., diffusion, viscosity, thermal conductivity) and the various space- and time-dependent correlation functions. Chapter 6 deals with extending MD from the traditional microcanonical (NVE) ensemble to both

the canonical (NVT) and isothermal-isobaric (NPT) ensembles. Chapter 7 covers non-equilibrium dynamics related to transport properties with emphasis on viscous flow, heat transport, and shear viscosity. Chapters 8 and 9 treat the dynamics of rigid molecules (the ubiquitous water model is used) and flexible molecules (i.e., polymers), respectively. Chapter 10 considers those cases in which geometric constraints are applied to some internal molecular degree(s) of freedom. Chapter 11 addresses systems in which either long-range forces (handled by Ewald sums) or three-body interactions must be incorporated into the MD algorithm. Chapter 12 shifts to MD algorithms and applications in which the continuous potential-energy function (e.g., LJ) is replaced by simpler step functions such as the hard-sphere potential. In Chapter 13, the use of MD to study time-dependent phenomena in fluid dynamics is described via two specific examples: (i) flow of a fluid past a rigid obstacle; and (ii) convective flow driven by a temperature gradient. Chapter 14 describes techniques for adapting the MD approach to parallel (i.e., distributed) and vectorized computing. In Chapter 15, the author closes by eloquently surmising the future of MD simulations. Appendices A1–A5 contain, respectively, sections on allocating arrays, on organizing input data, on managing extensive computations, on utility functions (e.g., random-number generation), and on header files. Appendix A6 provides a list of global variables used in the book's MD programs. The book concludes with an extensive Bibliography, a convenient Index of Functions defined in the book's MD code, and an adequate Subject Index.

In summary, this book would be a worthwhile acquisition for almost any scientist even remotely interested in MD simulations. The lucid writing style of the author lends itself to easy comprehension of even the most obscure technical concepts. The figures and tables, although few in number, are helpful in conveying the subject matter. If such an expression applies to a technical book of this kind, it was truly a pleasure to read. It is recommended highly, without qualification.

William J. Welsh
Department of Chemistry
University of Missouri-St. Louis
St. Louis, MO 63121 (USA)