

Book Review

**Advanced Computer Simulation Approaches for Soft Matter Sciences
I. Advances in Polymer Science, 173 Edited by Christian Holm and
Kurt Kremer (MPI für Polymerforschung, Mainz). Springer: Berlin,
Heidelberg, New York. 2005. xii + 276 pp. \$149.00. ISBN 3-540-22058-5.**

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Modern Techniques for Characterizing Magnetic Materials. Edited by Yimei Zhu (Brookhaven National Laboratory). Springer: New York. 2005. xx + 600 pp. ISBN 1-4020-8007-7.

This book provides an excellent resource for graduate students, postdoctoral researchers, and academic and industrial scientists across the many areas of research in magnetic materials. It comprises 14 chapters, each dealing with a particular magnetic measurement technique and is organized into five sections dealing with neutron scattering, X-ray scattering, electron scattering, scanning probe microscopies, and magneto-optical methods. Emphasis is placed on both newly developed and emerging techniques, e.g., spin-polarized scanning tunneling microscopy and time-resolved Kerr microscopy, as well as established and widely applied measurements, such as triple axis neutron spectroscopy, small-angle neutron scattering, and Brillouin light scattering. The inclusion of an entire section devoted to powerful resonant synchrotron X-ray techniques is noteworthy.

The contributors to the book have been carefully selected and in each case are highly cited experts of the particular method of magnetic characterization being discussed. Even the chapters dealing with established measurement techniques provide examples of the application of the technique to problems of contemporary interest. The chapters on the use of Brillouin light scattering as a probe of localized spin-wave modes in ferromagnetic nanostructures (Hillebrands) and the investigation of magnetic superlattices with perpendicular magnetic anisotropy using resonant X-ray techniques (Kortright) are excellent examples. The approaches such as those taken by Fitzsimmons and Majkrzak in the chapter on polarized neutron reflectometry guarantee a fresh coverage of a method that has been reviewed and summarized previously. In this chapter, the authors provide a "how to" guide to the acquisition and analysis of neutron reflectometry data (in addition to an exposition of the theoretical underpinnings), which is sure to be an invaluable resource to researchers new to the technique. It is important to note that each chapter is accompanied by a substantial bibliography composed of approximately 50 to 180 up-to-date references. A broad spectrum of techniques for magnetic characterization are covered, ensuring relevance to a wide range of scientists and engineers working in disparate subfields. The book covers techniques applied to magnetic nanostructures (the various microscopies, small-angle neutron scattering, etc.) and magnetic heterostructures (polarized neutron reflectometry, resonant X-ray scattering, Brillouin light scattering, etc.) as well as many forms of bulk magnetic materials of current interest (e.g., triple axis neutron spectroscopy).

In summary, *Modern Techniques for Characterizing Magnetic Materials* is a carefully selected compilation of descriptions of techniques for characterizing magnetic materials written by excellent contributors. It is likely to be a useful resource to a

wide audience across the chemistry, physics, and materials science of magnetic materials.

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Advanced Computer Simulation Approaches for Soft Matter Sciences I. Advances in Polymer Science, 173. Edited by Christian Holm and Kurt Kremer (MPI für Polymerforschung, Mainz). Springer: Berlin, Heidelberg, New York. 2005. xii + 276 pp. \$149.00. ISBN 3-540-22058-5.

Computer simulation is becoming an increasingly popular and powerful tool in the arsenal of engineers and scientists. This book contains four review articles by prominent experts in their fields that provide a broad range of physically relevant examples involving complex fluids, illustrating the type of molecular-level insights accessible via computer simulation. Simulation results are ultimately validated against experiment. While the authors make these necessary comparisons, they also make insightful connections to theory, which is important since approaches involving simulation and theory are complementary. This is one of the strong points of the book.

Chapter 1 is a well-written overview of outstanding issues in the theory and simulation of polymer solutions. The authors provide recent simulation-based developments in a number of areas, including phase behavior, interfacial properties, and nucleation. The second chapter focuses on thermostat algorithms, i.e., methods for maintaining more or less constant temperature, in computer simulation. Although this is an important technical issue, which highlights some of the nontrivial aspects of simulation, the topic does not fit within the general theme of this volume. Despite this, a welcome addition to Chapter 2 would have been a discussion of barostat algorithms. The phenomenon of interest in Chapter 3 is homogeneous and heterogeneous crystal nucleation in colloidal systems. The authors, generally speaking, provide a comprehensive review of the most recent computational, experimental, and theoretical developments in this subject. Last, Chapter 4 focuses on structure in polymer melts and blends. In particular, the chapter is devoted primarily to molecular dynamics (MD) simulation of polymeric systems and includes a concise summary of various molecular models, as well as an in depth discussion of PRISM theory. While MD is typically the method of choice when simulating complex molecules, noticeably absent from this chapter was a discussion of Monte Carlo methods of simulation.

From the title, one would expect substantial discussion of "advanced computer simulation" approaches. At the time these reviews were originally written, the simulation methods mentioned in them were perhaps state-of-the-art. However, in light of relatively recent methodological advances, this is no longer the case. Transition-path sampling and flat-histogram methods

are two examples of techniques that were not discussed, although the latter was mentioned briefly in passing in Chapter 1 along with successive umbrella sampling. This is certainly not entirely the fault of the authors but rather a reflection of how fast computer simulation is progressing. Finally, on a more superficial level, the book contains a significant number of editorial errors, e.g., grammatical, spelling, bibliographic, and mathematical, which made reading difficult at times.

On the whole, the book provides numerous examples of problems amenable to study via computer simulation. Although the simulation methods discussed in the book would not be considered "advanced" by present standards, they nevertheless remain quite powerful. Nonexpert simulators would no doubt benefit from reading through the examples. From a scientific perspective, this book should serve as a useful reference for those initiating theoretical or computational research in complex fluids.

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Dynamic Studies in Biology: Phototriggers, Photoswitches, and Caged Biomolecules. Edited by Maurice Goeldner (Université L. Pasteur Strasbourg, France) and Richard Givens (University of Kansas, USA). Wiley-VCH GmbH & Co. KGaA: Weinheim. 2005. xxviii + 558 pp. \$259.00. ISBN 3-527-30783-4.

There is increasing interest in using light to effect spatial and/or temporal control over chemical and biological processes. These goals challenge organic chemists to discover and develop selective and efficient photochemical reactions capable of generating useful molecules in a variety of matrices. This in turn has led to an exponential growth in the primary literature describing development and applications of photoreleasable protecting groups and other phototriggering strategies. Thus the appearance of this monograph, an attempt to summarize the literature up to approximately 2004, is quite welcome.

The book is divided into chapters that have been written by what appears to be a significant fraction of the experts in the field. In many cases, different sections of chapters have been written by different authors. In all, some 47 different coauthors have contributed to the monograph. The advantage of such an organization is that the various sections of the book are written by scientists having the greatest familiarity on a given topic. The disadvantage inherent in this approach is that there is bound to be some discontinuity in writing styles and unnecessary repetition of some topics. The editors have done a reasonable job at minimizing these problems.

As implied in the title, the monograph emphasizes biological applications of phototriggering technology. Thus there are chapters on very specific applications, such as the photoregulation of proteins and photocontrol of cellular processes. Two chapters cover the use of phototriggers in solid-phase synthesis and the fabrication of DNA microarrays. These latter two topics are not biology in the strictest sense, but they are certainly very relevant to biological research. There is also significant coverage of some of the basic photochemistry and reaction mechanisms involved in photorelease of substrates.

On the whole, I learned a lot by reading this book. The mix of fundamental chemistry and biological applications should make it an invaluable resource for any graduate student or researcher who hopes to enter this fascinating area of research. It does not aim to teach basic photochemistry, organic chemistry, or biochemistry, so I doubt it will find use as a textbook, outside of very specialized advanced courses. On the other hand, its excellent breadth of coverage and generally lucid descriptions make this book indispensable for any scientist who intends to develop or make use of phototriggers in biological systems.

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Functional Synthetic Receptors. Edited by Thomas Schrader (Philipps-Universität Marburg) and Andrew D. Hamilton (Yale University). Wiley-VCH Verlag GmbH & Co. KGaA: Weinheim. 2005. xii + 428 pp. \$180.00. ISBN 3-527-30655-2.

This is an interesting and engaging volume that summarizes work in the area of artificial receptors, broadly defined to include a range of topics from dynamic combinatorial libraries and molecular electronics to nucleic acid recognition. As such, it will appeal primarily to bioorganic and organic chemists as well as to those working in the area of organic materials. This breadth of subject matter is a strength of the volume and makes it enjoyable to read, both as a reference and as an opportunity to be exposed to a diverse range of topics. A challenge to the editors of such a volume, in which each chapter is written by a different author or group of authors, is to maintain a somewhat uniform style, both in content and in appearance. This allows the entire volume to exist as a cohesive exploration of the topic and not simply a disjointed amalgamation of random information. To this end, the editors Schrader and Hamilton have succeeded admirably.

The volume's figures are crisp and clear, although there are a few deviations from this, with pixelated images showing up on occasion. Overall the visual style is quite consistent, which makes reading the book easier. Each chapter stakes out a portion of the intellectual territory, e.g., "Molecular Containers in Action", "Synthetic Molecular Machines", "Carbohydrate Receptors", etc., and the authors then comprehensively assess the literature on the subject. A possible exception to this is the final chapter in the volume, "Replicable Nanoscaffolded Multifunctionality—A Chemical Perspective". It is primarily a theoretical/philosophical exploration about self-assembling nucleic acids. It includes "A Manifesto for Nanorobot Implementation" which makes for an interesting juxtaposition with the rest of the chapters, which consist of detailed examinations of more concrete issues, e.g., binding affinities and synthetic strategies.

Overall, the authors and editors do an excellent job of shaping a volume that covers a broad range of topics. The final product

nicely balances this breadth with enough depth to remain important and engaging.

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Modern Allene Chemistry, Volumes 1–2. Edited by Norbert Krause (University of Dortmund, Germany) and A. Stephen K. Hashmi (University of Stuttgart, Germany). Wiley-VCH Verlag GmbH & Co. KGaA: Weinheim. 2004. xvi + xii + 1143 pp. \$525. ISBN 3-527-30671-4.

This impressive two-volume set brings together more than two dozen authors to provide a superb description of allene chemistry and its applications, especially as applied to synthesis. Editors Krause and Hashmi note that nearly 8000 papers have been published on allene chemistry since the last broad review of this field two decades ago. The coverage thus focuses primarily on this period, with literature citations through 2004 in some chapters. Each chapter offers the best current review of the topic.

Volume 1 opens with four chapters on the synthesis of allenes. Specific chapters address isomerization routes to allenes, metal-catalyzed or -mediated reactions, and enantioselective allene synthesis. The second portion of this volume treats important structural types: allenic hydrocarbons, strained cyclic allenes,

donor- or acceptor-substituted allenes, and allenylmetal derivatives. Volume 2 begins with eight chapters on characteristic chemical reactions of allenes, including ionic and radical additions, oxidations, cycloadditions, cyclizations, and various aspects of metal-catalyzed allene chemistry. Throughout, the number of new synthetic applications is quite significant, especially those involving organometallic chemistry. A final four-chapter section covers “applications”, including allenic natural products (of which about 150 are now known!), pharmacologically active allenes, natural product synthesis involving allenic reagents, and enyne-allene chemistry. These topics are timely and well chosen, but missing is a chapter on applications in material science. There is also minimal coverage of higher cumulenes.

Allenes still receive scant attention in most general textbooks, although their importance in chemistry continues to grow. These two volumes are filled with novel chemical transformations and useful information that will stimulate further advancements in the field. Indeed, astute synthetic chemists will find many new reactions here to expand their chemical lexicon. This is not one of those book sets that should gather dust on the library shelves.

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