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BOOK REVIEWS

Molecular Nanostructures: XVII International Winterschool/Euroconference on Electronic Properties of Novel Materials. Edited by Hans Kuzmany (Universität Wien), Jörg Fink (Institut für Festkörper- und Werkstoff-Forschung, Dresden), Michael Mehring (Universität Stuttgart), and Siegmar Roth (Max-Planck-Institut für Festkörperforschung, Stuttgart). American Institute of Physics: Melville, New York. 2003. xviii + 640 pp. $215.00. ISBN 0-7354-0154-3.

This book was developed from the papers presented at the 17th International Winterschool/Euroconference on Electronic Properties of Novel Materials held in Kirchberg, Austria in March 2003. To quote the editors, contributions "focused on new nanostructured materials, with data presented on functionalized fullerenes and carbon nanotubes, non-carbon nanotubes such as BN and MoS_2 tubes, and new biological nanostructures." The book also covers "the direction of nanoelectronics research..., advancements in composite technology, and novel applications for nanotubes." There are 130 chapters, which are organized under the following headings: Fullerenes, Endohedrals, and Fullerides; Carbon Nanotructure Synthesis and Purification; Properties of Single-Wall Carbon Nanotubes; Characterization of Carbon Nanotubes; Functionalization of Carbon Nanotubes; Nanotube Filling and Double-Wall Carbon Nanotubes; Non-Carbonaceous Nanotubes; Theory of Nanostructures; Biological Nanostructures and New Materials; and Applications. An author index completes the book.

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Reviews in Computational Chemistry, Volume 19. Edited by Kenny B. Lipkowitz (North Dakota State University), Raima Larter (National Science Foundation, Arlington, VA), Thomas R. Cundari (University of North Texas), and Donald B. Boyd, Editor Emeritus (Indiana University-Purdue University at Indianapolis). John Wiley & Sons, Inc.: Hoboken. 2003. xxiv + 394 pp. $150.00. ISBN 0-471-23585-7.

The central theme of this latest volume of the series *Reviews in Computational Chemistry* is molecular and macroscopic modeling, and the common computational method that runs throughout all of the chapters is the Monte Carlo method. Thus, it is appropriate that the first chapter in this volume provides a good introduction to computational techniques and strategies for Monte Carlo methods. Although not exhaustive, the review focuses on strategies that are pertinent to modeling atomic and molecular clusters. The generalized metropolis Monte Carlo is the algorithm of choice by the authors, for it is widely used for computing thermodynamic properties of molecular systems. For systems that involve rotation to ensure that all possible orientations are sampled, the Barker−Watts algorithm based on the metropolis Monte Carlo procedure is described. Some practical considerations such as equilibration, estimating errors, and random number generation are discussed. Because systems that exhibit quasi-ergodicity are particularly challenging for most Monte Carlo methods, several techniques are introduced and described that can be used to overcome these difficulties.

Chapter 2 on hydrophobicity is particularly interesting and informative, challenging my understanding of the concept. One essential message of this chapter is that there must be consistency between experimental and theoretical results in defining hydrophobicity; surprisingly, convergence has not yet been achieved. Nevertheless, the chapter focuses on computational approaches and techniques that show promise toward providing insight into the origin of hydrophobicity at a molecular level. Similar methods are used to determine thermodynamic (free energy, entropy, and heat capacity) and structural properties of molecular systems displaying hydrophobic interactions. Such methods as the test particle thermodynamic integration and perturbation methods are introduced to the reader here.

Chapter 3 addresses the latest development in classical trajectory simulations. It starts with a review of the basic theory and the importance of analytical potential energy surfaces in performing such simulations. The innovation in this area is direct dynamics calculations. The use of mixed quantum mechanics and molecular mechanical theory as one approach for performing direct dynamics is described, and this is followed by a discussion of several examples, such as S_N2 reactions and surface-induced dissociation of protonated glycine.

Chapter 4 is a comprehensive review of the Poisson−Boltzmann equation, including an historical account of the equation and its deviation. Exact and approximate analytical solutions can be found for several systems (membrane, polymer, and micelle models), and numerical solutions to the equation are given. Moreover, a comprehensive list of over 700 references to the literature on the Poisson−Boltzmann equation is provided. This extensive chapter is a major contribution to the book.

Overall, this book covers an eclectic range of computational techniques in the area of molecular and macromolecular modeling. It is well written and should serve as a useful reference for both students and researchers in the field.

Joseph S. Francisco, *Purdue University*

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Biomolecular Films: Design, Function, and Applications. Surfactant Science Series Volume 111. Edited by James F. Rusling (University of Connecticut). Marcel Dekker, Inc.: New York, Basel. 2003. xii + 638 pp. $195.00. ISBN 0-8247-0899-7.

This book is intended to be "a modern collection of unique biomolecular film methodologies" and "techniques to investigate their properties". It includes topics such as the creation and analysis of biomolecular films and the use of biomolecular films

Unsigned book reviews are by the Book Review Editor.

in sensors and the synthesis of materials such as nanoparticles. The fabrication of biomolecular films and their characterization are covered in the first seven chapters, and the remaining five chapters are devoted to applications. The topics covered are wide-ranging, and each could easily justify a book on its own—in fact, there are good books on some of these topics currently available. The editor has managed to put together this collection of topics in a way that highlights the diversity of methods and applications in this field, and has very nicely met the stated goal of the text. One of the major strengths of this book is that it provides a concise, thorough review of the state of the broad field of biomolecular films.

The book contains 12 articles written independently by different authors who are experts in the field. As is to be expected in such a collection, the text is not as fluid in its presentation of the various topics or techniques as one would like. Specifically, useful information and references on a given technique are often scattered among several chapters instead of collected together. However, a good index of topics substantially mitigates this problem. The chapters are generally well written and provide the reader with an appropriate review of the topic at hand as well as insights into future goals and applications of a particular method or system.

The types of biomolecular films covered include lipid bilayers, self-assembled monolayers, DNA and protein layers, protein layers adsorbed on self-assembled monolayer films, and self-assembled multilayered films. Techniques for analysis that are discussed in detail include surface plasmon resonance, scanning electrochemical microscopy, and quartz crystal microbalance methods. A number of other commonly used techniques such as ellipsometry, IR spectroscopy, nonlinear optical spectroscopy, and atomic force microscopy are also covered, but in less detail. These discussions do not always provide enough detail for someone wishing to use the technique to learn the appropriate theory, although sufficient references are provided to the primary literature where that information can be found. This is certainly appropriate for a book with a scope as large as this one. Electrochemical methods of analysis and electrochemically active films comprise a disproportionate fraction of the material in this book. However, the editor and the authors have appropriately concentrated on their particular areas of expertise, and this does not significantly detract from the usefulness of the book.

The articles are generally accessible to beginning researchers in the area, but experts in the field should also appreciate the consolidation of all of these topics into a single book. This is a field that is currently quite active, and the authors have included a number of references to work over the past few years from laboratories other than their own. A number of the chapters in the book provide a significant amount of historical background as well as discussions of the theoretical basis for the techniques and methods used and their advantages and disadvantages. Review articles on many of these topics exist, but they are typically not as broad in scope as those in the present volume. It is certainly an extremely useful addition to the literature in this area, and I would highly recommend it to researchers interested in biomolecular films.

Cindy L. Berrie, *University of Kansas*

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