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BOOK REVIEWS

Molecular Devices and Machines: A Journey into the Nanoworld. By Vincenzo Balzani, Margherita Venturi, and Alberto Credi (Universita di Bologna). Wiley-VCH Verlag GmbH & Co. KGaA: Weinheim, Germany. 2003. xviii + 494 pp. $75.00. ISBN: 3-527-30506-8.

Much attention has been devoted in the past decade to the design, construction, and evaluation of a wide range of molecules that fall under the loose rubric of "Molecular Devices and Machines". The authors, who are major contributors to the field in their own right, have achieved a masterful overview of it. Coverage is extensive, and while the authors emphasize that they have made no attempt to be encyclopedic, this reviewer is unaware of any serious omissions.

The book is divided into three main sections: "I. Devices for Processing Electrons and Electronic Energy", "II. Memories, Logic Gates, and Related Systems", and "III. Molecular-scale Machines". The 16 chapters are heavily referenced, with most containing at least 100 citations, largely from the past 10 years, including a number from the first half of 2002. Where germane, coverage of naturally occurring systems (e.g., ATP synthase) is also included. The third section of the book ("Molecular-scale Machines") is essentially an updated but rewritten version of a review entitled "Artificial Molecular Machines" published in 2000 (Balzani, V.; Credi, A.; Raymo, F. M.; Stoddart, J. F. *Angew. Chem., Int. Ed.* **2000**, *39*, 3348−3391). Many of the very helpful schematic representations from the *Angewandte* review are repeated here, but presumably for economic reasons, without the full-color depictions that made the *Angewandte* review such a visual feast. The present volume contains a 15-page glossary that defines terms such as calixarene, hole transfer, and dynein for the nonexpert. There is no author index, but given a 16-page subject index and a seven-page Table of Contents, that absence is not a major deficiency.

It is noteworthy, albeit appropriate, that although virtually every molecule discussed had to be synthesized, often by very arduous sequences, the book does not discuss synthesis. Rather, it focuses on function and concept. Synthesis is "simply" the handmaiden that makes it all possible.

In summary, this inexpensive, attractively produced volume offers much, either for browsers seeking to acquaint themselves with a new field or for experts seeking a different perspective.

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Advances in Chemical Physics. Volume 127 . Edited by I. Prigogine (University of Texas at Austin and Université Libre De Bruxelles, Belgium) and Stuart A. Rice (University of Chicago). John Wiley & Sons, Inc.: Hoboken, NJ. 2003. x + 358 pp. $175.00. ISBN 0-471-23583-0.

Volume 127 of the *Advances in Chemical Physics* contains two chapters on unrelated topics in chemical physics, both of which are well-presented and should be of general interest to their corresponding communities.

In the first chapter, "Computational Strategies for Mapping Equilibrium Phase Diagrams", authors Bruce and Wilding discuss at various levels of detail several Monte Carlo sampling schemes that are widely used in the determination of the phase behavior of model substances. The mapping of boundaries for equilibrium phases requires knowledge of the differences in free energy between the given phases. The determination of these differences via molecular simulation is made difficult by the following problem: despite the dramatic increases in computational power over the past decades, an individual molecular simulation still samples only a small fraction of a system's relevant phase, or configuration, space. In general, the relevant configurations of each phase are typically "far" from each other, and thus multiple simulations are required to "link up" these regions of phase space. The calculation of the differences in free energy therefore requires that a suitable "path through configuration space" be chosen.

Bruce and Wilding present a well-balanced and up-to-date discussion of the various Monte Carlo sampling schemes, or different pathways through phase space, currently at the simulator's disposal. The methods discussed include, for example, serial and parallel sampling, extended sampling, thermodynamic integration, and phase switching. Their review is not exhaustive, at least from the point of view of detailing all the numerous examples and uses of the chosen techniques, though this is not, as the authors state, the purpose of their review. Rather, they provide a compact, highly informative, and well-presented introduction to the basic ideas and foundations of the various path-based sampling methods. They therefore focus on simple idealized model systems (an all-too-brief, in my opinion, subsection dealing with nonideal systems is given near the end of the chapter). Also included is a brief analysis of the advantages and disadvantages of each method. This is one of the many useful aspects of the authors' survey. I appreciated the authors' efforts to stress clarity of presentation. Many interesting and subtle aspects of sampling methods are discussed here, many of which have not been, until now, contained in a single review.

I hope, though, that the chosen title does not limit the readership of this chapter. As the authors state, the sampling techniques presented are not just applicable to the determination of equilibrium phase diagrams. Path-based sampling methods are relevant to other important problems, such as how free energy determines barriers for nucleation and the differences in free energies of conformations of polymers and proteins, and this excellent overview should be read by simulators working in these areas as well.

The second chapter of the book, "Molecular Models for Calculation of Dielectric/Far-Infrared Spectra of Liquid Water" by Gaiduk and Tseitlin, details the continuation of the authors' theoretical work (discussed previously in *Advances in Chemical Physics, Vol. 87*) in which the calculation of the dielectric/far-

infrared spectra of aqueous media, mostly liquid water, is now discussed (the previous work applied the authors' theoretical framework to strongly polar nonassociated liquids). This chapter contains an extensive and detailed overview comprising mostly the authors' work on this topic. Familiarity with the concepts and ideas presented in the previous review appears to be needed, however. Overall, the authors, both of whom have been working on this subject for quite some time, provide a detailed and comprehensive account of the molecular-based modeling that has been developed to obtain a theoretical understanding of dielectric responses in aqueous media.

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Reactive Intermediate Chemistry. Edited by Robert A. Moss (Rutgers University), Matthew S. Platz (Ohio State University), and Maitland Jones, Jr. (Princeton University). John Wiley & Sons, Inc.: Hoboken, NJ. 2004. viii + 1072 pp. $99.95. ISBN 0-471-23324-2.

This book of 22 chapters is divided into two parts: Part 1, "Reactive Intermediates" (16 chapters), and Part 2, "Methods and Temporal Regimes" (six chapters). The first part consists of reviews on specific intermediates by type: carbocations, carbanions, radicals, carbenes, etc., and the second part deals with techniques: matrix isolation, pulsed laser (nano,- pico-, and femtosecond) time-resolved spectroscopy, and theoretical methods. The reviews, averaging about 50 pages each, are up-to-date (extensively referenced to at least 2002), and most have a historical component that interweaves the older deductive approach with modern direct observational techniques and computational results.

This is truly an excellent book. The editors, all of whom have contributed to a chapter and are internationally known for their contributions to research, have a reputation as gifted scientific writers. The authors they have selected fall into the same category and were obviously carefully chosen; all are experts who write with clarity and a high quality rarely seen so uniformly through any text. Moreover, the graphics are also excellent, with a common format used throughout the entire book.

In the preface, the editors comment that it would be an ideal text for graduate students. I agree, although perhaps mostly but not necessarily, for students who have already been exposed to lower level, broader survey texts such as those by Carey and Sundberg, Lowry and Richardson, or Carroll. Particularly useful in this regard are the "Suggested Readings" that list important earlier reviews and precede the citations to the primary literature. However, the book is intended not only for graduate students but, perhaps even more so, as a resource that should be on the shelf of any practicing researcher who is a "student" of reaction mechanisms. I certainly learned a significant amount from every chapter I read.

Of course, one is expected to address deficiencies. In that regard, I can only comment that some readers will probably complain about minimal, or even lack of, coverage of their favorite reactive intermediate. The solution is obvious. A Volume II is required, and I encourage the current editors to proceed with that.

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