JACS
JOURNAL OF THE AMERICAN CHEMICAL SOCIETY

Subscriber access provided by ISTANBUL TEKNIK UNIV

Book Review

Reviews in Computational Chemistry, Volume 24 Edited by Kenny B. Lipkowitz (Howard University, Washington, D.C.), Thomas R. Cundari (University of North Texas, Denton), and Editor Emeritus, Donald B. Boyd (Indiana University-Purdue University, Indianapolis). John Wiley & Sons, Inc.: Hoboken, NJ. 2007. xxxiv + 518 pp. $175. ISBN 978-0-470-11281-6.

Richard K. Bowles

J. Am. Chem. Soc., **2007**, 129 (47), 14831-14831 • DOI: 10.1021/ja076992r

Downloaded from http://pubs.acs.org on February 9, 2009

More About This Article

Additional resources and features associated with this article are available within the HTML version:

- Supporting Information
- Access to high resolution figures
- Links to articles and content related to this article
- Copyright permission to reproduce figures and/or text from this article

View the Full Text HTML

ACS Publications
High quality. High impact.

Journal of the American Chemical Society is published by the American Chemical Society. 1155 Sixteenth Street N.W., Washington, DC 20036

J|A|C|S
BOOK REVIEWS

Reviews in Computational Chemistry, Volume 24. Edited by Kenny B. Lipkowitz (Howard University, Washington, D.C.), Thomas R. Cundari (University of North Texas, Denton), and Editor Emeritus, Donald B. Boyd (Indiana University-Purdue University, Indianapolis). John Wiley & Sons, Inc.: Hoboken, NJ. 2007. xxxiv + 518 pp. $175. ISBN 978-0-470-11281-6.

While confined fluids have been the focus of considerable interest for the past 20 years, the present text, subtitled "Nanoconfined Fluids: Soft Matter Between Two and Three Dimensions", is one of the first that is dedicated to reviewing the fundamental theoretical and computational aspects of the field. Unlike previous volumes of *Reviews in Computational Chemistry*, this one consists of a single monograph co-written by Martin Schoen and Sabine Klapp. However, the book's pedagogical style is very much in keeping with the philosophy of the series, and as such, it is a welcome and timely addition to the literature.

The true strength of this particular volume lies in its thorough development of the material. In the first two chapters, the authors take the interesting approach of presenting the thermodynamics and statistical mechanics of confined fluids within the context of strain and stress tensors, which are concepts usually reserved for the study of elastic solid bodies. This approach highlights one of the main characteristics that set these systems apart from bulk fluids and is a feature that is revisited in later sections that focus on the use of the isostress/isostrain ensemble in Monte Carlo simulations and the rheological properties of confined fluids.

Schoen and Klapp are interested in understanding the interplay of competing length scales, and this theme clearly plays out in the organization of the core Chapters 4−6, which focus on mean field theory, confined fluids with short range interactions, and systems with long range interactions, respectively. As the reader works through the text, it becomes clear how the molecular correlation length, confinement length scale, and, in the case of chemically heterogeneous substrates, the "chemical pattern" compete to give rise to a variety of unique liquid phases. I was pleased to see that the question of the thermodynamic stability and metastability of the respective phases was addressed, and again, this is shown to relate back to the relative importance of the various length scales. Furthermore, these chapters provide a good introduction to the main theoretical and computational techniques used to study confined fluids, although the book is not exhaustive in this respect.

The nature of the confining geometry is of central importance to the subject matter, and the authors generally use the ideal system of spherical particles confined in a slit-pore as their example. This is certainly beneficial with respect to the pedagogical goals of the text as it allows the different phenomena to be compared directly with respect to a simple model. The final chapter moves away from this and deals with the challenges associated with studying fluids confined within disordered materials. I would have liked to have seen the trend toward the study of more complex systems continued one step further to include some discussion of the confinement of molecules with complicated geometry, such as confined water, nonspherical molecules, or polymers. These systems are of considerable recent interest and introduce additional length scales of their own.

In closing, I found the text a pleasure to read. It is well written, and the mathematical development is clear and well supported with a number of appendices. The references are relatively up-to-date, and I would expect the book to be of considerable use to both newcomers to the field who want ready access to the key principles and theoretical/computational tools of the subject and more established researchers looking for a reliable, self-contained reference book.

Richard K. Bowles, *University of Saskatchewan*

JA076992R

10.1021/ja076992r

A Practical Guide to Magnetic Circular Dichroism Spectroscopy. By W. Roy Mason (Northern Illinois University). John Wiley & Sons, Inc.: Hoboken, NJ. 2007. xii + 224 pp. $125.00. ISBN: 978-0-470-06978-3.

Magnetic circular dichroism spectroscopy is a challenging area for students to understand both experimentally and theoretically. One of the real needs in this field has been a book that introduces it to senior undergraduates, beginning graduate students, and scientists wishing to learn more about the area. This monograph is an effort to meet this need.

After a short introduction, the book begins with a discussion of circularly polarized radiation, the basis for which many students often have trouble comprehending. Given the graphic capabilities today, additional illustrations would have been very useful here, as they would not only help clarify the concept of circular polarized radiation but could also help ignite the student's interest.

The next section introduces the theoretical framework of magnetic circular dichroism and provides some definitions of terms used in the field. Here and throughout the book, references are made to the book by Piepho and Schatz (Piepho, S. B.; Schatz, P. N. *Group Theory in Spectroscopy: With Applications to Magnetic Circular Dichroism*; Wiley-Interscience: New York, 1983). The following is a quote from the introduction: "The symbolism, definitions, and standard basis conventions of Piepho and Schatz are used here, so that if further elaboration of the mathematical development is required, the reader can easily consult the relevant sections of their book", which illustrates the biggest shortcoming of this book. The book by Piepho and Schatz has been out of print for a number of years and is therefore very difficult to obtain. Yet, it is referred to many times. Without the Piepho/Schatz book, you cannot see the extensive tables referred to or other information. Because this text is out of print, it would have

been better to include all the needed information in the book or give references to other available sources with the information.

The author then discusses the instrumentation of magnetic circular dichroism. It would have been interesting to see a discussion of the problems connected with the instrumentation for the various regions of the electromagnetic spectrum. The author's area of expertise is magnetic circular dichroism of inorganic complexes in the ultraviolet−visible region; thus, he is most familiar with the instrumentation and the interpretation of data for that region, which may have affected the overall coverage of the subject matter. For instance, he discusses using an iron complex for calibration, which is very useful in the visible region but is not a method used in other regions of the electromagnetic spectrum. References to all the calibration methods would have been very useful to someone entering the field.

The next section of the book gives short reviews of various papers published about magnetic circular dichroism spectroscopy. In my opinion, it would have been better if the author had given more details than the original paper rather than less. This would have meant fewer case studies, but this could have been addressed by giving more references to other publications, which also might have created the opportunity to allow for more references to recent publications in the field.

In conclusion, the author discusses polarized electromagnetic radiation, the theoretical framework of magnetic circular dichroism, instrumentation, and measurement and interpretation of magnetic circular dichroism spectra. He also provides a definition of terms used in the field as well as a discussion of magnetic linear dichroism spectroscopy. A dream book would capture both the students' interest and allow them to see the possibilities of the field. Although this is not quite the dream book this reviewer had hoped for, it is useful to introduce students and other scientists to the field. It is a pleasure to see an author willing to tackle this spectroscopic technique in a book, as it is not a trivial subject to present to beginning scientists in the area.

Patricia Ann Snyder, *Florida Atlantic University*

JA077004P

10.1021/ja077004p