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BOOK REVIEWS

Computational Chemistry of Solid State Materials: A Guide for Materials Scientists, Chemists, Physicists and Others. By Richard Dronskowski (RWTH Aachen, Germany). Wiley-VCH Verlag GmbH & Co. KGaA: Weinheim. 2005. vi + 294 pp. $125.00. ISBN 3-527-31410-5.

The science of solid-state materials has evolved over the past several decades into a multidisciplinary area combining elements of condensed matter physics, surface science, materials science, chemistry, and engineering. Most current researchers approach the field with a formal grounding in chemistry or solid-state physics. Whereas the physics of solid-state materials has become a well-developed field, its chemistry is a comparatively recent one. Since little or no formal training in solid-state chemistry is usually included at the undergraduate or even the graduate level, chemists rely heavily on the availability of secondary and tertiary literature sources. Until recently, this meant that the personal library of a typical solid-state chemist contained classic texts on solid-state physics with little or no sources that specifically focus on the chemical properties of solid-state materials. More recently, texts focusing on computational chemistry as a distinct discipline have begun to appear. It is in this context that Dronskowski has provided "Computational Chemistry of Solid State Materials".

The book is composed of three main chapters focusing on classical and quantum mechanical methods and another chapter covering some specific examples. The main focus is on inorganic materials with less attention devoted to molecular crystals. The chapter dealing with classical methods outlines the main aspects of Coulombic interactions between ionic species, in particular as pertains to lattice constant prediction. While the discussion of the Coulombic interactions is informative, the treatment would have benefited from a more expanded description of the Ewald method for modeling ionic lattices, which has become the method of choice in nearly all classical computational tools. In addition, there is little mention in this chapter of classical force-field methods for modeling solid-state materials. Such methods have come into widespread use for modeling large extensive systems, particularly where lattice defects and surface phenomena are of interest.

The second chapter covers the use of quantum mechanical methods and begins with a treatment of the solution of the many-body Schrödinger equation using the variational approach. The incorporation of solid-state effects, such as periodic boundary conditions and symmetry, follow. The treatment is essentially the same as that commonly found in solid-state physics texts: construct a reciprocal space lattice and form Bloch states as products of a reciprocal lattice plane wave and the atomic basis-set wave functions. The treatment is particularly valuable in subsequent sections in which these principles are applied to linear, planar, and three-dimensional lattices in which the concept of band structure is also introduced. This treatment is similar to that of Cox in "The Electronic Structure and Chemistry of Solids" (Oxford University Press), which ought to have been included in the bibliography. The author does a good job covering the intricacies of electron−electron interactions including exchange and correlation, which are often glossed over in introductory texts. An exception to this is the text of Hehre et al., "Ab Initio Molecular Orbital Theory" (Wiley), which would be another good companion to Dronskowski's. The latter part of this chapter touches on the use of molecular dynamics and structure optimization as well as the calculation of thermodynamic properties. Finally, the author has provided a listing of available computational code widely used by modern computational chemists.

In the third chapter, quantum and classical computational methods are illustrated for several materials of current technological interest. Particular attention is drawn to the advantages and drawbacks of the various methods. For example, predictions of relative stability of two possible crystal polymorphs can fail due to limitations in the method used. Specific examples, which are invaluable for those new to these techniques, are given where this can occur.

The book should be useful to graduate students and postdocs working in theoretical and computational solid-state chemistry as well as to solid-state experimentalists who want to incorporate computational methods into their research areas. For the former, the book is an accessible extension of graduate-level quantum mechanics to problems in the science of condensed matter materials. The examples given in the latter chapter are particularly informative in this respect.

A unique strength of the book is that the author presents the various methods from the context of problem-solving, with a fairly neutral perspective of the relative merits of each method. The book is highly readable and accessible for nonexperts and, along with other texts as noted above, should greatly enhance the training of anyone in this field.

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Annual Review of Physical Chemistry, Volume 57, 2006. Edited by Stephen R. Leone (University of California, Berkeley), Paul Alivisatos (University of California, Berkeley), and Ann E. McDermott (Columbia University, New York). Annual Reviews: Palo Alto, CA. 2006. xvi + 692 pp. $188.00. ISBN 0-8243-1057-8.

There are 20 chapters in this latest issue of Annual Review of Physical Chemistry, representing "a swath through the field of physical chemistry, much like a cut through a potential surface at a particular time in a reacting system" to quote from the preface. There are two prefatory chapters in this volume, the first by Jortner and the second by Hochstrasser giving their personal accounts of the people, places, and experiences that influenced their lives in science and drove their research to what

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it is now. The remaining 18 chapters cover a range of topics in physical chemistry from Zewail's study of "4D Ultrafast Electron Diffraction, Crystallography, and Microscopy" to Schinke et al.'s "Dynamical Studies of the Ozone Isotope Effect: A Status Report". A subject index, a cumulative index of contributing authors, Volumes 53−57, and a cumulative index of chapter titles 53−57 complete the book.

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Anion Receptor Chemistry. By Jonathan L. Sessler (University of Texas, Austin, USA), Philip A. Gale (University of Southampton, UK), and Won-Seob Cho (University of Texas, Austin, USA). From the Series: Monographs in Supramolecular Chemistry. Edited by J. F. Stoddart. Royal Society of Chemistry: Cambridge. 2006. xvi + 414 pp. $219. ISBN 0-85404-974-6.

In 1997, the field of anion receptor chemistry was established enough for the publication of an edited text by Bianchi, Bowman-James, and Garcia-Espana. That text is wide in scope and includes discussions of the thermodynamics and theory of anion binding, natural anion receptors, and the structural and topological aspects of synthetic anion binding, as well as various applications, including catalysis, in the use of anion receptors. In the decade since then, the science of anion recognition and its resulting applications have continued to mature as evidenced by the publication of many reviews, including such serial reviews as *Topics in Current Chemistry, Volume 255* (2005) on anion receptors and sensors and *Coordination Chemistry Reviews, Volume 240* (2003) on synthetic anion receptor chemistry.

Unlike the above publications, this monograph by Sessler, Gale, and Cho is intended to provide a work that is "more pedagogical in nature" and is "geared to those coming into the field for the first time, either as...[a] graduate-level chemistry student or as an established researcher." With a rather narrow scope, it eschews theory and instead focuses on the authors' selected examples of the structure of anion receptors. In this, the work is organizationally and conceptually different from the monograph edited by Bianchi et al. In Chapters 2−7, the authors describe in great detail anion receptors that contain charged organic functional groups, neutral functional groups, and metal-containing receptors; receptors that bind both anion and cation as ion pairs; and their own work on expanded porphyrin and elaborated porphyrinogen anion receptors. Unfortunately for a pedagogical work, the writing in these chapters is very dense. The work is inadequate in its use of tables, except for the chapters covering the authors' own work. Instead, the text is filled with numerical equilibrium constants in such numbers as to become almost soporific. This might not be such a problem if the chapters were better organized to compare those receptors within each structural category that were best at binding spherical, linear, trigonal, or tetrahedral anions, as is done in the above-mentioned edited text and serial reviews. Instead, the organization of these chapters relies mostly on receptor functional groups.

Chapters 6−9 are well presented and a joy to read. The examples presented in Chapter 6 illustrate well the approaches several researchers have taken for the preparation of receptors that effectively bind ion pairs. In Chapters 8 and 9, the authors provide cogent examples of the uses of anion receptors in sensors or as templates in the controlled assembly of large systems. Where this work really shines is with the authors' inclusion of a multitude of X-ray crystal structures of receptor−anion complexes throughout the text, most of which are in color. The topology of receptor−anion complexes is clearly presented, providing excellent illustrations of the structural requirements for potent anion binding.

The monograph is not exhaustive in its presentation of anion receptor chemistry. However, for those interested in more examples of anion receptors, further applications involving anion receptor use, or receptor synthesis, the authors include an extensive reference section at the end of each chapter for the reader's perusal. While I am not convinced that this monograph would work as a textbook, the authors did a very credible job in providing a solid reference text on anion receptor chemistry.

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Optical Chemical Sensors. Edited by F. Baldini (IFAC-CNR, Florence, Italy), A. N. Chester (Hughes Research Labs, Inc., Malibu, CA), J. Homola (IREE-Academy of Sciences, Prague, Czech Republic), and S. Martellucci (The University of Rome "Tor Vergata", Italy). Springer: Dordrecht. 2006. xxxii + 536 pp. $99.00. ISBN 1-4020-4609-X.

This book is based on the Proceedings of the NATO Advanced Study Institute on optical chemical sensors held in Erice, Sicily in late July and August, 2004. The opening chapter, or lecture, is an introduction to the history of masers and lasers, and the second gives a historical overview of fiber optic chemical sensors and biosensors. The fundamentals of optical chemical sensors and their applications are covered in the remaining 23 chapters. A short subject index completes the book.

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