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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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