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BOOK REVIEWS

Computational Inorganic and Bioinorganic Chemistry. Edited by Edward I. Solomon (Stanford University, Stanford, CA), Robert A. Scott (University of Georgia, Athens), and R. Bruce King (University of Georgia, Athens). John Wiley & Sons, Ltd: Chichester. 2009. xx + 594 pp. $220. ISBN 978-0-470-69997-3.

In many regards, the past decade has seen the emergence of computational chemistry in all sectors of chemistry. Computational chemistry may rightly take its position next to such techniques as NMR spectroscopy and X-ray crystallography as an indispensible tool in the elucidation of chemical systems and processes. Historically, the application of modeling to inorganic chemistry problems has lagged behind that of the organic realm with respect to the quantity and quality of simulation tools. The gap between inorganic and organic applications has narrowed greatly, and the present volume highlights the state of the art in computational inorganic chemistry.

The editors of this book have amassed a veritable "who's who" of the computational inorganic chemistry community to write a series of chapters, more than three dozen in all, split up into three sections: Methods; Case Studies - Bioinorganic; and Case Studies - Inorganic. There is much to like about this volume, which is very comprehensive, although not all-encompassing, which I will explain later. First and foremost, the editors have sought input from experts in areas of methodology in addition to the reigning champion, density functional theory (DFT). While one may argue whether DFT should or should not stand for "Damn Fine Theory," it is clear that the F does not stand for "Foolproof". Indeed, there are many quantum and classical modeling techniques that may be profitably applied to inorganic chemistry, if used judiciously. Hence, widening the scope of this book to include both DFT and non-DFT methods is admirable. Further in this vein, one might hope that neophytes, perhaps attracted to computational chemistry by the alluring siren call of B3LYP, might happen upon this volume and see that there exist many other modeling techniques, each with advantages and disadvantages, that may be profitably used in the modern research enterprise. As a result, introducing readers here to the many fruits of the theoretician's labor, e.g., semiempirical quantum mechanics, multiconfigurational quantum mechanics (written by the late Bjorn Roos), molecular mechanics, and so forth, is an endeavor worthy of pursuit, and in this regard, the editors have done a splendid job.

Another strong suit of this volume is the generous focus on analytical techniques and fundamentals in computational inorganic and bioinorganic chemistry, e.g., bonding and structure analyses, functional/basis set selection, spectroscopic property calculation, etc. Such attention is essential for going beyond calculated numbers to the fundamental chemistry that lies "under the hood", so to speak. Moreover, it is the analytical portion of the computational exercise, which admittedly can be tedious, that is typically needed to answer the most common question one gets from novices to computational chemistry: How much should one trust these calculated results? Readers of this book can look through the numerous case studies, find one or more that best suits their predilections, and obtain a virtual apprenticeship by seeing how the experts enlisted by the editorial team go about analyzing their own results.

Another positive aspect of this book is the wide range of "elemental" coverage. In computational inorganic chemistry, the right tool or tools for the job is often intimately linked to what portion of the periodic table one is dealing with. For example, computational solutions appropriate for light main-group elements may or may not work for heavy s-block elements, and d-block metals can, and often do, require different modeling strategies from their f-block cousins. Within this volume, coverage is given to transition-metal chemistry, main-group chemistry, noble gas compounds, metals and nonmetals, and lanthanides and actinides.

For the aforementioned reasons, this book is broad in scope and covers a topic of interest to many in the chemical community. However, *Computational Inorganic and Bioinorganic Chemistry* is not all-embracing in its coverage of areas of application. One area is glaringly absent. If one tried to make a short list of such areas that drive much of current research in inorganic chemistry, biological applications and catalysis would certainly be expected by most to be on such a list, and indeed, within the case-studies portion of the book, these areas deservedly receive considerable attention. If I were to find fault with this book, it would be in the lack of coverage of applications in inorganic materials chemistry and the lack of focus on methodology. Few things have been as actively pursued in the past decade by chemists as the desire to incorporate the prefix "nano" into many of our research endeavors. However, there is little emphasis in this volume on modeling strategies that would be pertinent to modeling in the inorganic materials arena. Performing quantum calculations on solid and extended systems, novel force fields that can model reactive entities or empirical potentials for metal/alloy modeling, heterogeneous catalyst modeling, multiscale modeling, and modeling at the mesoscale and continuum scale are but a few areas that could have been incorporated into this book.

Overall, *Computational Inorganic and Bioinorganic Chemistry* is a first-rate effort. The editors have assembled an impressive team of experts from across the globe to introduce the current status of computational inorganic chemistry to a larger audience. With the exception of a lack of emphasis on case studies in materials chemistry, coverage of topical areas is large and impressive. Furthermore, those with an interest in main-group, transition-metal, and f-block chemistry can find useful information to inform and guide their own modeling efforts. Likewise, the decision to go beyond discussion of DFT approaches is commendable. In short, I would think that this volume would be useful to a wide portion of the chemical community from novice experimentalists who may wish to dip their foot in the pool to full time modelers who seek to wade in deeper waters.

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