Book Review

Reviews in Computational Chemistry, Volume 21 Edited by Kenny B. Lipkowitz (North Dakota State University), Raima Larter (Indiana University-Purdue University), and Thomas R. Cundari (University of North Texas). John Wiley & Sons, Inc.: Hoboken, NJ. 2005. xxviii + 443 pp. $150.00. ISBN 0-471-68239-X.

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This 21st volume in a long and well-regarded series continues the tradition of expert, timely reviews of active areas of research in computational chemistry, broadly defined. Computational chemistry is a rapidly changing field and one in which the leading edge of the scientific literature is often only accessible to the narrowly focused expert. By contrast, the articles in *Reviews in Computational Chemistry* are targeted to readers with some background in chemistry and computational methods and are designed to inform them about the state-of-the-art in each focus area and provide useful pointers into the current research literature. They are particularly useful for the computational chemist in one subfield (e.g., a quantum chemist), either new or experienced, who would like to learn about another subfield in computational chemistry (e.g., chemoinformatics).

This tradition is alive and well in this current volume. The first review, by Dovesi et al., on ab initio quantum simulations of interest in solid state chemistry is a particularly readable treatment of the issues that arise in performing quantum simulations of crystalline materials. Typically, quantum chemists deal with single molecules, often organic, using orbital-based methods, whereas the minority of quantum chemists, and majority of quantum physicists and materials scientists, who work with crystals use plane-wave or other methods optimized for periodic systems. This article succeeds in bridging the gap between these two approaches. The authors focus on one particular package, their own CRYSTAL code, but provide pointers to other available codes.

The next three reviews could be broadly categorized as dealing with aspects of chemoinformatics. The first of these, by Bultinck et al., concerns the concept of molecular similarity, specifically, how the similarity of two molecules can be quantitatively determined, based on quantum mechanical calculations. Both the definition of quantum molecular similarity and the application of this approach in areas such as quantitative structure/activity relations (QSARs) are described. The next article, by Faulon et al., is a comprehensive account of the ways in which graph theory can be used to enumerate molecules, an important step in screening the molecules via a QSAR for some useful functionality. Several examples of the successful use of this approach are provided in this review. The third contribution in this group, by Livingstone and Salt, addresses the issue of reducing the number of variables used in a multivariable QSAR and similar applications to a set of relatively independent and useful variables. As in the previous two articles, many of the examples of the application of this method relate to computer-aided drug design.

The article by Baker is an introduction to the use of Poisson−Boltzmann methods to model the electrostatic interactions in biomolecular simulations. In such simulations, the computational cost of using explicit electrostatics can be prohibitive; hence, the application of Poisson−Boltzmann theory to determine effective interactions becomes of interest, although the geometry within which the resulting partial differential equations must be solved is complex, defined by the surface of the biomolecule, and invites discretization using state-of-the-art gridding methods. In addition to the underlying theory and discussion of issues associated with discretization, the author provides pointers to commercial and public-domain solvers. The final review in this volume by Aguda et al. concerns computational methods for deducing models for gene regulatory networks (GRNs), a rapidly growing subfield of systems biology made possible by the enormous amount of information coming from high-throughput experiments. A GRN refers to a set of molecules and interactions that affect gene expression, and a model for a GRN is a set of first-order differential balance equations encapsulating these interactions. Computer-aided generation of GRN models from data collections has been a long-term goal of systems biology, and the present article is a description of progress toward this goal.

In summary, this volume of *Reviews in Computational Chemistry* contains readable and accessible reviews of six different areas of computational chemistry. A practicing computational chemist will find something interesting in each of them, as well as a good foundation for learning more about each topic. Hence, this monograph will be a fine addition to any institutional library and could be a welcome addition to the personal library of anyone wanting to keep abreast of the ever-expanding reach of computational chemistry.

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