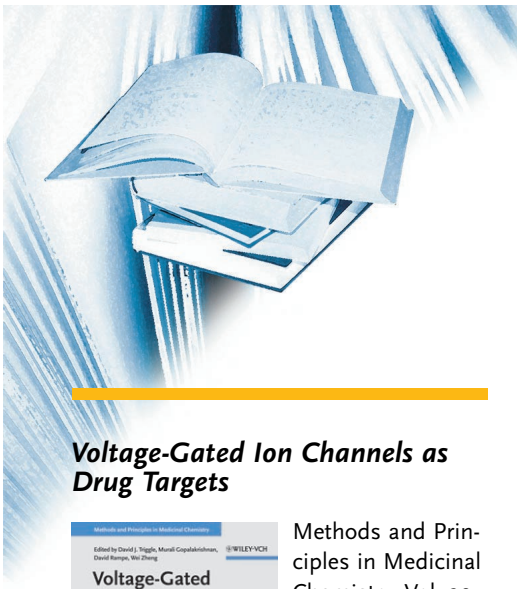
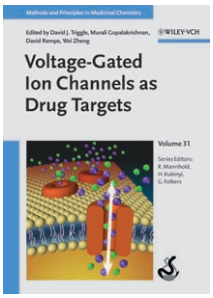


Voltage-Gated Ion Channels as Drug Targets



Methods and Principles in Medicinal Chemistry, Vol. 29. Edited by *David J. Triggle*, *Murali Gopalakrishnan*, *David Rampe* and *Wei Zheng*. Wiley-VCH, Weinheim 2006. 480 pp., hardcover € 149.00.—ISBN 3-527-31258-7

Ion channels are important targets for medicinal chemistry. Nifedipin, Diltiazem, and Verapamil are prominent examples of established drugs that act on heart-associated calcium channels, and are used for the treatment of hypertension and angina pectoris. This monograph is a comprehensive collection of articles about voltage-gated ion channels and known drugs that interact with these channels. All the contributing authors are well-recognized experts in the field.

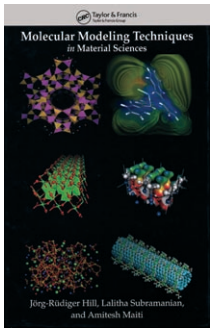
The book consists of eight chapters (479 pages). After a brief general introduction to ion channels (Chapter 1), the superfamily of voltage-gated ion channels is summarized by W. A. Catterall in Chapter 2. Chapter 3, by S. I. McDonough and B. P. Bean, focuses on state-dependent drug–channel interactions. Chapter 4, by D. Leishman and G. Waldron, describes the electrophysiological techniques (e.g., the patch clamp) for investigating ion-channel function and drug-mediated modulation of the function. Many chemists do not have a background knowledge of electrophysiology, and for them this chapter is very helpful. The following three chapters on ion channels (Chapter 5, calcium channels, by C. Doering and G. Zamponi; Chapter 6, sodium channels, by D. S. Krafte, M. Chapman, and K. McCormack; Chapter 7.1, potassium channels, by M. Gopalakrishnan, C.-C. Shieh, and J. Chen) present information on channel subtypes, channel structure, ligand sites, and drugs that are active at the channel. For each drug the chemical structure, binding affinities, and references are given. Lastly, Chapter 8, by K. Bracey and D. Wray, deals with genetic and acquired channelopathies. Every chapter or subchapter has its own list of references. A subject index rounds off the book.

The book is written for medicinal chemists who seek information about specific ion channels and their drugs. Biophysicists or biochemists who are interested in structure–function relationships are not the main target audience. Other books, such as that by Hille (*Ion Channels of Excitable Membranes*, *3rd ed.*, Sinauer Associates, Sunderland, 2001) will contribute supplementary knowledge for those readers. But even for them, *Voltage-Gated Ion Channels as Drug Targets* provides an up-to-date literature overview.

The present book will be indispensable for all libraries of pharmaceutical companies. University libraries and researchers with an interest in the subject will also certainly wish to acquire this book.

Philipp Reiß, Ulrich Koert
Fachbereich Chemie
Universität Marburg (Germany)

Molecular Modeling Techniques in Material Sciences



By *Jörg-Rüdiger Hill*, *Lalitha Subramanian* and *Amitesh Maiti*. CRC Press/Taylor & Francis 2005. 328 pp., hardcover $ 111.50.—ISBN 0-8247-2419-4

Molecular-level modeling of materials has grown tremendously in the past 15 years, and today simulation has firmly joined experiment and theory as the third major branch of scientific methods in materials research. This growth has been driven by exponential increases in computer speed, by development of powerful new modeling algorithms and software, and by the need for more detailed molecular-level understanding of the high-tech materials of today and tomorrow. *Molecular Modeling Techniques in Material Sciences* is a timely addition to the growing literature on molecular-level modeling of materials.

The stated goal of the book is "to provide an overview over commonly used methods in atomistic simulation of a broad range of materials, giving enough theoretical background to understand why, for example, a certain type of forcefield may be applied to a zeolite while the same may not work well for glasses. Or why the local density approximation may be used for geometry optimization of a semiconductor structure while it is not used to predict the band gap of the semiconductor". The focus is entirely on microscale modeling, including electronic structure calculations and force-field modeling such as Monte Carlo and molecular dynamics (MD) simulations.

The first chapter of the book provides an introduction to the scope of molecular modeling, followed by a qualitative overview of quantum-chemical and force-field modeling techniques. Mathematical and other details of the computational methods are delayed to the last chapter of the book. The terse

overview of the simulation methods in Chapter 1 will be difficult reading for anyone new to the field, but I imagine that many people will not read the book straight through anyway. The chapter also provides a nice section on available software (both commercial and some academic) for molecular modeling.

Chapters 2–6 cover the main classes of materials considered in the book: metal oxides, microporous materials, glasses, semiconductors and superconductors, and nanomaterials. The book explicitly excludes polymers, and there is very little on metals. Many of the chapters include longer discussions of examples from the literature that give specific insights obtained from molecular modeling. This might include how modeling helped interpret experiments or provided information that would be very difficult to measure with direct experiments. These case studies are then followed by additional examples that list the properties calculated and the techniques employed, but give little additional information. This combination of depth and breadth keeps the book interesting and informative, while limiting it to a reasonable number of pages. The book contains 879 literature references altogether, and most sections include abundant references to the original literature, with an emphasis on work published in the past 10 years. A few sections lack references to relevant review articles and monographs that would also be helpful to newcomers to a topic. Chapters 2 through 6 are the heart of the book, and distinguish this book from others focused more on methods and less on applications to materials.

Chapter 7 provides a 93-page overview of computational quantum chemistry, force fields, Monte Carlo simulations, and MD simulations. This treatment is too brief to enable someone to learn this material well enough to develop codes, but it may be enough for someone planning to use commercial software. It does provide a good review of key concepts and equations, and there are some good insights in these pages, even for experienced practitioners. The appendices include a useful list of abbreviations, basis set naming conventions, and atomic units.

Occasionally, in Chapters 1 and 7, it seems that the authors have tried to condense things too much and have inadvertently introduced statements that might be misleading. For example, in Chapter 1, after a discussion of energy-minimization techniques, the authors write: "If one is interested in the behavior of a material at a finite temperature, one needs to perform a so-called 'molecular dynamics' simulation". But this is not exactly true, because one could instead perform a Monte Carlo simulation. Similarly, in Chapter 7 the verbal description of the acceptance rules for grand canonical Monte Carlo simulations is not strictly correct (and unfortunately no references are given). There are a few other minor errors in the book, such as missing units in a few tables, but for a book of this length the number of errors is admirably low.

I imagine this book will be especially useful to researchers doing molecular modeling in industry. A successful industrial molecular modeler must be a "jack-of-all-trades", and does not have the luxury of specializing in one type of technique or one particular type of material. In a company that may have only one or two researchers dedicated to molecular modeling, these researchers must often deal with systems that are new to them, and this book is nicely organized for readers who want to focus in quickly on a topic of interest. This organization should also be appreciated by academics moving into a new area of materials modeling. With appropriate supplementary resources, new graduate students will also find the book useful.

This book should be a welcome and useful addition to university and industrial libraries. It provides a quick entry into appropriate methods and literature examples for modeling a variety of materials, and this subject is sure to gain in importance in the coming years.

Randall Q. Snurr
Department of Chemical and Biological Engineering
Northwestern University
Evanston, IL (USA)

DOI: 10.1002/anie.200585358