

not be suppressed for very long." Thus, according to Kuhn, for true scientific revolutions to occur, the system must eventually respond to those who think "outside the box" or "outside the paradigm". One learns from studying the history of science that the scientific process assumes that its entire structure is contingent on the arrival of another structure that does everything the current one does, and more. However, the history of science also teaches that one must be prepared to get things wrong, and that there are mechanisms in the scientific process for eventually bringing to light errors in extraordinary claims. The larger the error of the extraordinary claim, the more there is at stake, and the greater the need to identify the error quickly. Progress in science requires a balance between the conservatism imposed by the prevailing paradigms and the necessary skepticism for new ideas, and the liberalism of new ideas that smack of paradigm shifts. The tension between thinking inside the box and thinking outside the box is an essential tension without which scientific progress would languish. For the reader who would like to pursue the subject further several references are provided.^[2-6]

Whether or not you agree with Park's take on voodoo science, a message of the book is that if scientists do not take a more significant role in the way that science is disseminated to the public and especially to politicians, voodoo science will continue to survive. The book is an easy read and will probably be a source of enjoyment to some who see in Park's examples situations that resonate with their own experiences. However, the book may be a source of irritation to others who are not entertained by a polemical point of view. I strongly recommend that you give it a try to see how it fits your particular tastes concerning how science works (or doesn't).

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Molecularly Imprinted Polymers. Man-Made Mimics of Antibodies and their Applications in Analytical Chemistry. Edited by *Börje Sellergren*. (Series: Techniques and Instrumentation in Analytical Chemistry, Vol. 23.) Elsevier, Amsterdam 2000. 557 pp., hardcover \$ 301.00.—ISBN 0-444-82837-0

"Intelligent polymers", "polymers with memory", and "artificial antibodies" are some of the descriptions often applied to molecularly imprinted polymers (MIPs). These are inorganic or organic materials that are prepared by polymerization with cross-linking in the presence of templates, which may consist of small molecules, biopolymers, microorganisms, or crystals. On removing the template one obtains a specifically molded polymer which is a negative image of the template. The origins of the technique go back 80 years, but it is only very recently that the method has become widely used, and publications on the subject are now appearing with a near-exponential growth rate.

This book edited by Börje Sellergren consists of 21 chapters, many of which are contributed by the leading experts in their special fields. It begins with a very interesting historical overview, which is followed by a brief description of the physicochemical fundamentals of the molecular imprinting process. The next ten chapters describe in detail the different methods for preparing MIPs and the special polymerization techniques used. The remaining eight chapters are concerned with applications of MIPs in analytical chemistry, for example in chromatographic investigations. Four of the chapters are devoted to the rapidly developing area of chemosensors based on MIPs.

The book comes close to fulfilling the editor's claim that "this book provides the first complete coverage of the area of molecular imprinting". However, the focus on analytical chemistry as indicated in the title means that not all aspects are covered. Applications in organic synthesis and in catalysis would certainly have provided material for another special chapter, in view of the many publications on these aspects that have appeared. For readers who are already working in the area of molecular im-

printing or intend to do so, the many technical details and the extensive bibliography (over 1400 references!) will be of great interest. On the other hand, those who only seek an initial overview of the technique should instead read some of the shorter reviews (e.g., G. Wulff, *Angew. Chem. Int. Ed. Engl.* **1995**, *34*, 1812).

With such a large international team of authors it would be difficult to avoid some overlapping of subject matter, and unfortunately this book has not escaped that problem. Many research results are described in several places. Also some of the introductions to individual chapters are unnecessarily detailed and redundant. For example, on page 396 the difference between covalent and non-covalent imprinting is explained yet again with diagrams, even though that topic was covered in detail at the beginning of the book in two chapters of over 100 pages in total. It is especially annoying when two chapters with a partly shared authorship contain whole passages of text that are nearly identical (pp. 196 and 286; pp. 197 and 290).

In a first edition of a book with almost 600 pages, there are inevitably a few small mistakes. Examples are the duplication of one of the figures (pp. 299 and 300) and the highly unsuitable abbreviation Me for a metal ion (p. 199). However, the book can be recommended for all readers interested in gaining a detailed and up-to-date survey of the fascinating technique of molecular imprinting.

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Quantum-Mechanical Prediction of Thermochemical Data. Edited by *Jerzy Cioslowski*. Kluwer academic publishers, Dordrecht 2001. 251 pp., hardcover \$ 90.00.—ISBN 0-7923-7077-5

The book provides an excellent survey about recent approaches towards highly accurate ab initio methods for the prediction of thermochemical data, which is very useful for theoretical chemists and certainly worth the price. The editor

Jerzy Cioslowski has invited international theoreticians to summarize the various computational schemes, ranging from strict *ab initio* theory with powerful parametrized schemes to semi-empirical approaches.

Chapter 1 by Helgaker et al. describes *ab initio* studies of simple molecules at extremely high levels of theory. As demonstrated and discussed in detail, these methods allow the prediction of atomization energies with rather remarkable accuracies close to or even within the error bars of experiment. These authors also discuss frankly the limitations of the methods used, of which the major one is that only small molecular systems of first-row elements can be treated with the highest accuracy. In Chapter 2, Martin and Parthiban introduce the Weizmann theories W1, W2, and their variants. In an admirable manner, the authors guide the reader from the development of basic concepts to various applications, and also pay attention to limitations in accuracy as well as computational costs. Furthermore, the authors find a nice balance between correct theoretical formalisms and understandable wording, making it a pleasure to read not only because of scientific content. Chapter 3 by Raghavachari and Curtiss is dedicated to Gaussian theories (Gn) and their variants, of which the latest version G3 yields chemically accurate thermodynamics at moderate computational expenses. Unfortunately, the authors concentrate on the advantages of the Gn methods, but hardly mention problematic cases nor compare the Gn schemes to the related Wn and CBS methods. The complete basis set (CBS) scheme is introduced by Petersson in Chapter 4. The CBS methods qualify as capable competitors of Wn and Gn theories from both a *a priori* approach as well as the performance, and certain CBS variants can also be used to accurately describe larger molecules. In fact, the author applies the CBS method to an example from enzyme catalysis and concludes: "This is an exciting time for computational science."

In Chapter 5, we leave the "chemically accurate" methods and turn to more approximate schemes. The electron propagator method described by Ferreira et al. offers a computationally

efficient routine for the calculation of various properties, but the error margins are rather large and systematic improvement seems to be difficult within the approximations used. The value of the method is the prediction of ionization energies and excited states of larger molecules. A brilliant example of applied quantum chemistry is provided by Henry and Radom in Chapter 6, which deals with the thermochemistry of substituted alkyl radicals. For this purpose, the Gn-RAD schemes were developed which are variants of the respective Gn methods particularly adopted for the description of open-shell species. Moreover, the authors provide extensive data for comparing the various theoretical approaches including the Wn and CBS methods as well as density functionals, thus allowing their performances to be evaluated with respect to relative and absolute energetics as well as activation parameters. Therefore, their contribution is ideally suited for experimentalists interested in the reliability of different theoretical approaches. Transition metal chemistry is dealt with in Chapter 7 by Fröhlich and Frenking. As stated, the authors focus on their own results and present lots of data, but provide limited general insight. Moreover, most of the compounds are almost or completely coordinatively saturated, such that the typical, sometimes dramatic problems encountered in the theoretical description of transition metal compounds do not become evident. Considering the relevance of transition metals in catalysis, and likewise the formidable challenge these compounds present for *ab initio* theory, the book might have improved further by a second contribution on this topic. Last, but not least, Thiel summarizes the present status of semi-empirical methods in Chapter 8. While these methods became somewhat suppressed by the vast development of *ab initio* methods (and of computers) within the last decade, semi-empirical methods still represent the "working horse" in theoretical applications to life science. Further, Thiel introduces orthogonalization procedures which offer prospects for further improvements of semi-empirical schemes.

In summary, all chapters summarize the status of specific branches of contemporary computational chemistry

from the viewpoints of the authors. The contributions have adequate lengths and are sufficiently referenced. Two drawbacks remain in my view. Firstly, density functional theory is mentioned several times but not discussed explicitly, even though DFT and its hybrid variants are among the most frequently used methods nowadays; a separate chapter might have been adequate. Secondly, the book lacks some kind of more general evaluation of the various methods. In fact, I expected such a missing link when reading the title "Theoretical Thermochemistry: A brief survey" in the Table of Contents. The disappointment is even greater when it turns out that the correct title of Chapter 8 is "Semiempirical Thermochemistry: A brief survey".

As far as the potential readership is concerned, the book is primarily regarded useful for computational practitioners, but also newcomers will find a good introduction into the repertoire of contemporary theoretical methods for thermochemical predictions.

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Electrochemistry of Nanomaterials.

Edited by Gary Hodes. Wiley-VCH, Weinheim 2001. xvi + 340 pp., hardcover € 152.00.—ISBN 3-527-29836-3

The physical properties of nanoscale materials have been the subject of intense experimental and theoretical study in recent years, and exciting new applications ranging from novel electronic devices to biological sensors continue to emerge as the field expands. In this context, the term nanoscale often refers to systems that are sufficiently small in at least one dimension that they exhibit properties that are strongly size-dependent. In this case, the energy levels for electrons are affected by quantum confinement, so that optical and electronic properties can be tuned by size selection. Quantum-well structures (small in one dimension) are a long-established feature in the physics of semiconductor devices, whereas applications for quantum wires (small in two dimensions) and