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 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 practioneers, but also newcomers will find a good introduction into the repertoire of contemporary theoretical methods for thermochemical predictions.

Detlef Schröder
Institut für Chemie
Technische Universität Berlin (Germany)

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

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quantum dots (small in all three dimensions) are more recent. In spite of the nonclassical limit that this classification of nanomaterials implies, systems that are not small enough to show quantum confinement effects are also commonly referred to as "nanoscale". This wider definition has been adopted by Gary Hodes when assembling the component chapters of this book, which are written by authors actively pursuing research on the electrochemical synthesis and application of nanoscale materials.

The physics and chemistry of nanoscale materials is a rapidly developing area, so that any book dealing with these topics runs the risk of being out-of-date by the time it is published. At the same time, it is clearly impossible for a book to be comprehensive. Nevertheless, it is disappointing that several important topics have been omitted from this compilation. For example, one would have expected a chapter outlining the fascinating work on the electrochemistry of metal nanoparticles by Schiffrin, Murray, Wilner, and others. Similarly, there is little discussion of the electrodeposition of nanowires. Readers expecting a systematic approach to nanoscale materials will not find it in this book. Instead, Gary Hodes has collected a number of individual essays representing a selection of topics in the field indicated by the title of the book.

Penner opens the book with a comprehensive and well-written account of synthetic routes to nanoparticle arrays based on electrochemical deposition of metallic precursors. The discussion illuminates the advantages and disadvantages of a combined electrochemical/chemical approach compared with chemical routes to nanoparticles on substrates. By contrast, the following chapter by Hodes and Rubinstein gives a less clearly defined overview of electrodeposition of semiconductors that fails to address the central question: why use electrochemical methods for synthesis? Readers familiar with the extensive literature dealing with size-selective chemical preparation methods may find it difficult to see what electrochemistry has to offer. The next chapter by Switzer establishes a sharper goal-orientated focus. The comprehensive discussion of the electrodeposition of two- and three-dimensional structures explains clearly the synthetic objective of the work, and shows how it relates to better-established nonelectrochemical techniques such as molecular beam epitaxy. The next two chapters deal with the electrochemical preparation of porous semiconductors. Kelly and Vanmaekelbergh summarize their work on porous compound semiconductors such as GaP, and Green, Létant, and Sailor give a rather brief account of the preparation and properties of porous silicon. Much of this work has been discussed more comprehensively elsewhere. The two chapters that follow both deal with nanocrystalline systems, with particular reference to dye-sensitized nanocrystalline solar cells. Lindquist and co-authors focus on charge transport in nanostructured films, and their chapter is well researched with an extensive bibliography. By contrast the chapter by Cahen and co-authors on dye-sensitized cells is more self-referential and ignores a substantial body of more recent work. The very substantial overlap in terms of subject matter between these two chapters is surprising, and it demonstrates the lack of interaction between authors during the preparation of the book. The final chapters by Kamat (electrochromic and photoelectrochromic aspects) and by Cassagneau and Fendler (self-assembled ultrathin films) are competent and up-to-date reviews. That by Cassagneau and Fendler is a pleasure to read, since it communicates a feeling for a dynamic and expanding area that will clearly make a real impact in terms of new technology.

After reading this book, I was left with the impression that its chapters had come together by a process of self-assembly. The lack of thematic structure and the absence of editorial influence inevitably detract from the intrinsic importance of the topics covered. A glance at the list of symbols (listed for each chapter at the end of the volume) reveals a series of errors and inconsistencies. The Faraday constant becomes Faraday's number; film thickness is variously L, d, D, and even W. This inconsistent collection of symbols and definitions is likely to confuse readers and set a poor example to graduate students. Perhaps publishers should make editors more aware of the important role that they can play in eliminating such inconsistencies and errors. In spite of these deficiencies, this book is an excellent source of information and a good introduction for readers who wish to know more about the way in which electrochemistry is contributing to the rapid evolution of nanoscale materials and systems.

Laurence Peter
Department of Chemistry
University of Bath (Great Britain)

Combinatorial Library Design and Evaluation. Edited by *Arup K. Ghose* and *Vellarkad N. Viswanadhan*. Marcel Dekker, New York 2001. 631 pp., hardcover $ 195.00.—ISBN 0-8247-0487-8

This book contains 20 articles by authors from both industry and academia, arranged in four parts. Part 1 consists of a very informative introduction which explains the basic principles of the design of small molecule libraries. Part 2 consists of six articles dealing with the principles of modeling pharmacophores, establishing quantitative structure–activity relationships, molecular docking methods, and the broad topic of scoring functions. Part 3 contains eight articles on topics of current interest in the area of library design. These include detailed discussions of knowledge-based methods, the concept of "drug-likeness", different measures of diversity, special algorithms for virtual screening, combinatorial approaches, and various current ideas for defining and measuring "molecular similarity". Lastly, Part 4 consists of five articles dealing with some special methods and with the practical application of the methods described in the preceding chapters.

Special emphasis is given to the recent trend of using different computer-aided methods in combination, and also the integration of these into strategies for searching for new pharmacologically active agents. Reading the book gives one a clear appreciation that a single method is often insufficient for success, and that in most cases a combination of several molecular descriptions and methods of classification and virtual screening is more likely to achieve the

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