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BOOK REVIEW

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Book Review of Metallic Systems: A Quantum Chemist's Perspective

Metallic Systems: A Quantum Chemist's Perspective. Edited by Thomas C. Allison (National Institute of Standards and Technology, Gaithersburg, MD), Orkid Coskuner (The University of Texas, San Antonio), and Carlos A. González (NIST, Gaithersburg, MD). CRC Press (an imprint of Taylor & Francis Group): Boca Raton, FL. 2011. xvi + 404 pp. $149.95. ISBN 978-1-4200-6077-5.

This book covers topics in computational chemistry with applications to M-containing drugs, catalysts, and enzymes (M = metal atom); metal ions in aqueous solutions; M_n clusters ($n < 10$, $n < 100$ for M = Au); surfaces of metal oxides; and liquid and solid metal surfaces.

It is not possible to cover something as vast as "metallic systems" in one book, but some important topics are noticeably absent, e.g., bulk metals and their alloys; metal atoms and clusters embedded in solids; nanoclusters in the scalable size regime (M_n, $n \approx 100-10^6$); and metallic solids made of main group elements, such as O_2 under extreme pressure or conducting polymers. This partly has to do with the format of the book: there are 11 chapters, and most of them emphasize the authors' own research contributions. Some are reviews, some are partial reviews of others' work and partial summaries of articles by the authors, and a few are almost in the style of an original contribution, with little review material. The cited work makes up for the lack of breadth somewhat, with many useful leads into the literature. There are over a thousand references, and roughly 200 of them are works published in the period from 2007 to 2010.

The book includes a mix of theory, approximations, and computational methods, on one hand, and discussion of the chemistry and physics of metallic and metal-containing systems, on the other. The first four chapters feature short descriptions of hybrid quantum-classical ("QM/MM") and Molecular Dynamics (MD) methods and case studies showing how calculations give insight into solvated metal ions and metal-containing catalysts, drugs, and biomolecules. Chapters 5−7 are about the surfaces of liquid metals, solid metals, and metal oxides, with emphasis on physics in Chapter 5 and on practical aspects of computational modeling in Chapters 6 and 7. The remaining four chapters cover applications to small metal clusters. Chapters 8 and 9 have detailed descriptions of the tight-binding approach and of a Gaussian-based implementation of Density Functional Theory (DFT), respectively. Applications to Au_n and transition metal clusters illustrate these methods. Chapters 10 and 11 are shorter and deal mainly with the geometric and electronic structure of selected small clusters.

After many years of collective effort to improve theoretical methods, metallic systems remain challenging. Errors on calculated energy differences can be 10 kcal/mol or even more for small systems. Simulation protocols with seemingly minor differences can give qualitatively different results. There are no generally accepted models or methods for metals. DFT and MD are often used, but there are many implementations that differ in the details, and the details matter. Several interesting examples in the book show that, with due attention to details and careful validation of computational models, one can successfully tackle tough problems that go beyond the structure and thermodynamic properties of gas-phase species, such as mechanisms of catalytic reactions, solvation of metal ions and M-containing species, the geometric and electronic structure at the metal−vacuum interface, and magnetic and optical properties of clusters. No book has sure-fire recipes for those types of calculations, but this one has many good pointers for researchers who want to understand, or contribute to, the literature on the theory of metallic systems.

In general, the book is long on modeling strategies, computational details, and illustrative calculations and short on fundamentals and principles. The state of the art ca. 2009 is described, but that is rapidly changing. My main criticism is that the chapters and sections are very uneven in format, style, and quality, and they do not interconnect very well. Some sections look out of place and relate only indirectly to metals or quantum chemistry. There is a theme that runs through the book, however: details in computational models and methods matter, and complex questions about metallic systems can be answered if proper attention is given to these details.

The book is at a level accessible to PhD students and researchers with basic knowledge in theoretical physical chemistry. Individuals may be interested in some of the chapters, but not all of them, and chapters can be read in any order. I recommend this book as a worthwhile addition to a science library.

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