Design of Heterogeneous Catalysts

As the editor states in the Preface, heterogeneous catalysis will serve a critical role in society's quest for a clean planet, stable economy, and a renewable energy future. These goals will rely heavily on processes that utilize highly active and selective heterogeneous catalysts. However, current methods of catalyst synthesis do not produce materials active and selective enough to fulfill this role. An emphasis within fundamental catalysis research is the determination of structure–function relationships, but often structurally ill-defined materials are used, reducing the utility of these relationships. A small (but growing!) fraction of researchers have identified that new methods for catalyst design and synthesis are required for heterogeneous catalysis to serve the role the editor envisions. The book demonstrates that the inspiration for catalyst design comes from many sources, including bio-inspired (or biomimetic), self-assembly, and guided first-principles computational approaches. Synthetic methods to control the composition and structure of the active site, as well as the local environment around the active site, are discussed by experts in the field.

In 12 chapters, the book covers topics on the synthesis, characterization, and modeling of catalytic materials. The synthesis of catalytic materials dominates, but each chapter contains sufficient information on the characterization of the materials, as well as an evaluation of their catalytic performance. The chapters "Optimal Design of Hierarchially Structured Porous Catalysts" and "Theory-Aided Catalyst Design" demonstrate the effectiveness of complete computational approaches in catalyst design, while the chapter "Design of Bimetallic Surfaces" shows that catalysts predicted by theory to be more active and selective can be synthesized and their superior catalytic performance verified experimentally.

Many chapters complement each other well, and it would have been appropriate if the editor had made a statement connecting them or juxtaposed the relevant chapters. For example, the chapter "Optimal Design of Hierarchially Structured Porous Catalysts" discusses the design of pore networks to increase effectiveness factors for diffusion-limited reactions by designing catalysts with bimodal pore distributions. In Chapter 12, an experimental method—dual templating—for the synthesis of porous bodies containing bimodal pore-size distributions was introduced, yet the connection between the two chapters is not made. There is also some repetition in the book, with separate chapters containing identical information. For example, Chandler et al. report on the use of dendrimers in catalyst design, including the ability of dendrimers to template and stabilize reduced metal nanoparticles, while in the chapter "Self-Assembled Materials for Catalysis" Zhu et al. discuss the same topic in less than a page. In light of the chapter devoted entirely to dendrimers in catalyst synthesis, it is apparent that this section in Zhu's chapter is redundant and unnecessary.

There is only one chapter solely dedicated to the characterization of heterogeneous catalysts, which was disappointing when one acknowledges the fact that advanced tools for characterization must be developed concurrently to complement new methods of catalyst synthesis. These techniques must be energy, temporally, and spatially resolved to enable the development of rigorous and robust structure–function relationships. However, this chapter on in situ X-ray absorption spectroscopy (XAS) techniques for the characterization and design of catalysts is well-written, and the authors nicely integrate the current state-of-the-art with the future of XAS in catalysis science.

The editor combines new materials and concepts with classic topics in catalyst synthesis. A very informative chapter on open metal frameworks and their application in heterogeneous catalysis was a nice introduction to the topic, as well as a chapter on the synthesis of catalytic nanostructures that mimic biological nanomotors. This reviewer was a bit disappointed that there was no chapter dedicated to the synthesis of molecular heterogeneous catalysts based on the grafting of organometallic compounds. This is a mature area in catalyst design and inclusion of such a topic would have made for a more complete book.

Overall, the book is composed of a nice selection of chapters written by authorities within their respective discipline. This book should find a home on the bookshelf of chemical engineers, chemists, and materials scientists, especially those whose focus is on the synthesis of catalytic materials. I hope the editor and publisher agree to publish a follow-up to *Design of Heterogeneous Catalysts* because this is a rapidly growing field with new developments occurring almost daily.

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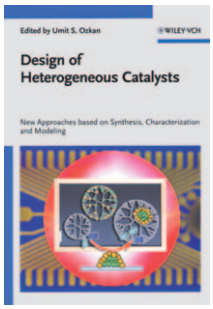

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