**Molecular Catalysts: Structure and Functional Design**

**Edited by Lutz H. Gade and Peter Hofmann**

Molecular catalysis is an exciting field and one in which there has been rapid development in recent years. This book, edited by Lutz Gade and Peter Hofmann, aims to highlight a wide range of different aspects of the study of molecular catalysts, from high-level quantum-chemical studies of fundamental mechanistic steps to catalysis in synthesis, catalyst immobilisation for large-scale industrial applications and the understanding of structure and function in enzymes. It does so through a series of case studies, many of which focus on the excellent work that has been done over the last ten years or so in Heidelberg’s Collaborative Research Centre on molecular catalysis. The book is likely to appeal to both newcomers to the field, who will benefit from the specific insights of each case study and from understanding the methodological approaches that are being used in the area, and also to more experienced researchers in catalysis.

The book opens with a highly engaging foreword by Roald Hoffmann, which elegantly reminds us of some of the historical aspects of catalysis and the fact that even seemingly simple reactions, such as the platinum-catalysed oxidation of hydrogen, have taken many years of study to understand – and that aspects of this reaction still remain mysterious. The subsequent chapters are separated into five key parts:

Part I focuses on mechanistic studies that have delivered fundamental insights into elementary processes of relevance to a range of catalytic reactions. This includes fascinating computational work, including quantum-dynamical studies on olefin insertion into an M–H bond and its reverse process, β-hydride elimination, and investigations into the reactivity of clusters of metals or metal oxides isolated in inert gas matrixes. The potential for single-molecule fluorescence spectroscopy to be used as a tool for understanding homogeneous catalytic processes is discussed in one chapter. In others, an overview of recent developments in our understanding of highly synthetically important gold catalysis and a discussion of diastereoselectivity in alkene metathesis are very clearly presented.

Part II highlights the fact that, while the discovery of new, unprecedented catalytic reactions is a highly active and successful aspect of current research, and is providing valuable new synthetic methodologies (e.g. in organic synthesis), the optimisation of existing homogeneous catalytic reactions (e.g. hydroformylation, hydrocyanation, hydrosilylation and others) is also very important and has the potential to significantly impact many key industrial processes. One of the key themes of this part of the book is the use of ligand design, where possible driven by mechanistic understanding, to modify catalyst properties in order to develop more active, selective or stable catalytic systems.

Part III discusses catalysis in synthesis. A range of examples are included, but there is a particular focus on asymmetric catalysis and the development of one-pot sequential catalytic reactions. As with the chapters in part 2, ligand design is important here, but the focus in this part is on the novel synthetic applications that become possible through the use of modern catalytic reactions.

Part IV is concerned with the study of catalysis in biological systems, specifically in enzymes such as cytochrome P450cam and hybrid catalysts based on a combination of homogeneous catalysts and nucleic acid biopolymers. These and related systems are of great interest from a fundamental perspective, but also have significant potential in the development of novel catalysts that are bio-derived or bio-inspired. As with other chapters, there is a strong interplay between experimental and computational studies in evidence in this part of the book.

The book concludes with part V, which presents three chapters on supported catalysts and high-throughput screening of catalytic reactions. The immobilisation of molecular catalysts on various types of support has the potential to combine the desirable properties of both homogeneous and heterogeneous catalysis and some novel approaches to this, such as dendrimer supports for stereoselective catalysis and solid-supported biomimetic catalysts, are reviewed here. A very interesting chapter describing the use of on-column reaction chromatography for in situ kinetic analysis completes part V.

Overall this book gives a very enjoyable overview of many aspects of the highly diverse field of catalysis, as viewed through the lens of the Heidelberg Collaborative Research Centre on molecular catalysis. I am very happy to recommend it to aspiring or established researchers in this area.