## Fundamental Concepts in Heterogeneous Catalysis

Heterogeneous catalysis is without doubt a key technology in chemical industry world-wide. The steady decrease in reserves of fossil fuels makes this subject even more important, since new catalysts are needed to convert sunlight energy (from the point of view of mankind, the only "endless" energy source) into a variety of chemicals in an efficient, sustainable, and environmentally friendly way, and to do so on a large scale to satisfy the ever-growing need for energy. The challenge is enormous, and inspiration-driven progress might not be enough. A more fundamental and holistic approach based on reliable theory is needed. This is precisely the point of view underlined by the authors of this book, which, in 12 short chapters, presents a significant part of the current knowledge of the mechanisms of heterogeneous catalysis, from an atomic- and molecular-scale perspective, including a focus on applications, and touching on aspects of catalysis engineering. This is accomplished by relying on a thorough analysis of energy and free energy profiles obtained from density functional theory (DFT) based calculations on appropriate, mostly periodic, surface models, a field to which the authors have made important contributions.

Following a brief introductory chapter, Chapter 2 introduces the important concepts of adsorption, reaction, and activation energy at surfaces, describing the roles of the surface plane and of low-coordinated sites. Several complicated concepts, such as zero-point energy and partition function, are introduced in a pedagogically effective way. Some of these concepts and remarks are highlighted in boxes throughout the text, a feature that graduate students will certainly appreciate.

Next, the authors briefly review some concepts of chemical equilibrium. Here the authors use some expressions which, from a purist point of view, deviate from a rigorous formalism of the thermodynamic potentials involved. However, the reader is warned that these are approximations. From a practical viewpoint, and for the authors' main purpose, these are sufficiently accurate. Statistical thermodynamics (in a simplified form) is used to show how the computed DFT energies can be used to predict thermodynamic magnitudes and relationships; for instance, the derivation of a Langmuir isotherm is simple and beautiful.

Chapters 4 and 5 are devoted to the problem of predicting and using rate constants. The authors admit that they have chosen to develop this in a rather technical way; that is certainly true, although the formal part can be skipped without losing a comprehensive overview. The different presentations and concomitant approximations of transition state theory give a useful insight. These two chapters also introduce orders of magnitude for the main quantities, which are often lacking in more general textbooks; this is an important and useful piece of information, especially for computationally orientated readers.

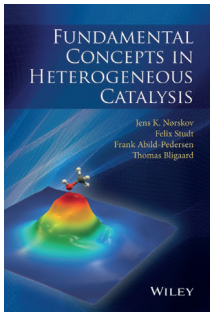
Chapter 5 introduces and illustrates the useful concepts of descriptors and of scaling and Brønsted–Evans–Polanyi relationships, which largely reflect outstanding results and accompanying interpretation from the authors' own research. In the next chapter, descriptors are used to derive activity maps and, more importantly, selectivity maps; these invaluable tools allow screening of different catalysts without a high computation cost, thus adding a predictive power to the overall approach.

The physical basis for the scaling and other relationships is given in Chapter 8, where the well-known d-band model developed by some of the authors is described in detail. This provides a link between the band theory of solids and the qualitative concepts of the chemical bond. A more elaborate picture is developed at the end of the book (Chapter 12), including additional details on band theory, the Newns–Anderson model, and its application to understand trends in bond adsorption energy.

Up to this point, the discussion of results is limited to those obtained from DFT calculations for perfect, flat, or stepped surfaces. To consider more realistic catalyst models, structure and support effects are discussed in Chapter 9. This introduces concepts such as the degree of structure sensitivity, and the effects of the support and promoter, thus providing a useful tool to obtain information about the physical nature of the active site, which is needed when attempting to design new catalysts or to improve existing ones. The effects of promotion and poisoning are described very briefly in Chapter 10.

Chapter 11 tackles a subject that is hot and difficult: surface electrocatalysis, which is one of the most promising technologies for energy production. Here, the authors describe in detail the latest knowledge gained from the theoretical simulation of reactions taking place at electrode surfaces, in which they generalize most of the concepts and tools introduced in the previous chapters, and describe in detail the similarities and differences between the two environments. The book is completed by Chapter 12, already mentioned above.

This monograph offers a comprehensive description of the state of the art in the field of theoretical heterogeneous catalysis, with the emphasis on deriving broad trends rather than on the particular accuracy of the DFT calculations




**Fundamental Concepts in Heterogeneous Catalysis**
By Jens K. Nørskov, Felix Studt, Frank Abild-Pedersen and Thomas Bligaard. John Wiley and Sons, Hoboken 2014. 208 pp., hardcover, € 83.70.—ISBN 978-1118888957

carried out. This differs from some mainstream works on quantum chemistry, which aim at precise prediction of the thermochemistry. For the complex systems involved in heterogeneous catalysis, reaching a predictive description already constitutes a big step. For readers who want a deeper insight, the book includes a number of appendices that provide some more detailed discussion of several key points, and some selected references, including many from the authors' publications. The text is perhaps somewhat biased towards a solid-state-physics point of view, with concepts that might not be familiar to readers with a chemistry background. However, it is certainly a valuable complement for chemists working in the area of heterogeneous catalysis and aiming for a deeper knowledge of the magic hidden in catalysts.

*Francesc Illas*
Physical Chemistry Department
University of Barcelona (Spain)

**International Edition: DOI: 10.1002/anie.201506018**
**German Edition: DOI: 10.1002/ange.201506018**