DESCRIPTION

This practical guide describes the basic computational methodologies for catalysis and materials science at an introductory level, presenting the methods with relevant applications, such as spectroscopic properties, chemical reactivity and transport properties of catalytically interesting materials. Edited and authored by internationally recognized scientists, the text provides examples that may be considered and followed as state-of-the-art.

ABOUT THE AUTHOR

Rutger Anthony van Santen gained his doctorate in theoretical chemistry in 1971 from the University of Leiden, joining Shell Amsterdam as a research chemist the following year. In 1988 he became Professor of Catalysis at the Eindhoven University of Technology, where he was promoted to scientific director in 1989. In 1991 he became director of the Netherlands Institute of Research in Catalysis, and in 2005 he was made Royal Netherlands Academy of Science and Arts Professor. He is a member of the Royal Dutch Academy of Arts and Sciences, Dutch Academy of Engineering and is a Knight in the order of the Dutch Lion. Professor van Santen has been active in many national and international catalysis research programs and organizations. He is the author or editor of 13 books, over 600 research papers and 22 patents, and has been awarded several national and international awards and visiting professorships. His main research interest is the molecular mechanistic understanding of catalytic reactions.
Philippe Sautet was born in 1961, has studied at Ecole Polytechnique in Paris and defended his doctorate in Theoretical Chemistry at Orsay University (Paris XI) in 1989. He then entered CNRS at the Institute of Research on Catalysis in Lyon, where he set up developed and led a group devoted to the applications of theoretical chemistry to heterogeneous catalysis. He is now Director of research at CNRS, and director of the Laboratory of Chemistry at the Ecole Normale Supérieure of Lyon and at CNRS. He has published over 150 scientific papers.

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