DESCRIPTION

The Nobel Prize in Chemistry 2007 awarded to Gerhard Ertl for his groundbreaking studies in surface chemistry highlighted the importance of heterogeneous catalysis not only for modern chemical industry but also for environmental protection. Heterogeneous catalysis is seen as one of the key technologies which could solve the challenges associated with the increasing diversification of raw materials and energy sources. It is the decisive step in most chemical industry processes, a major method of reducing pollutant emissions from mobile sources and is present in fuel cells to produce electricity. The increasing power of computers over the last decades has led to modeling and numerical simulation becoming valuable tools in heterogeneous catalysis.

This book covers many aspects, from the state-of-the-art in modeling and simulations of heterogeneous catalytic reactions on a molecular level to heterogeneous catalytic reactions from an engineering perspective. This first book on the topic conveys expert knowledge from surface science to both chemists and engineers interested in heterogeneous catalysis. The well-known and international authors comprehensively
present many aspects of the wide bridge between surface science and catalytic technologies, including DFT calculations, reaction
dynamics

on surfaces, Monte Carlo simulations, heterogeneous reaction rates, reactions in porous media, electro-catalytic reactions, technical
reactors,

and perspectives of chemical and automobile industry on modeling heterogeneous catalysis. The result is a one-stop reference for theoretical

and physical chemists, catalysis researchers, materials scientists, chemical engineers, and chemists in industry who would like to broaden

their horizon and get a substantial overview on the different aspects of modeling and simulation of heterogeneous catalytic reactions.

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**ABOUT THE AUTHOR**

Olaf Deutschmann studied physics in Magdeburg and Berlin. In 1996, he obtained his doctoral degree (chemistry) from Heidelberg University supervised by Jürgen Warnatz. He then worked on high-temperature catalysis at the University of Minnesota with Lanny D. Schmidt and at the Los Alamos National Laboratory. After receiving the venia legendi in Physical Chemistry at Heidelberg University he joined the University of Karlsruhe in 2003. Today, he holds the Chair in Chemical Technology at the Karlsruhe Institute of Technology (KIT), Germany, and is speaker of the Helmholtz Research School Energy-Related Catalysis. His group works on heterogeneous reactions for the synthesis of chemicals and materials, reduction of pollutant emissions, and energy conversion. He is recipient of the DEHEMA Award of the Max Buchner Research Foundation and of the Hermann-Oberth-Medal in Silver.

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