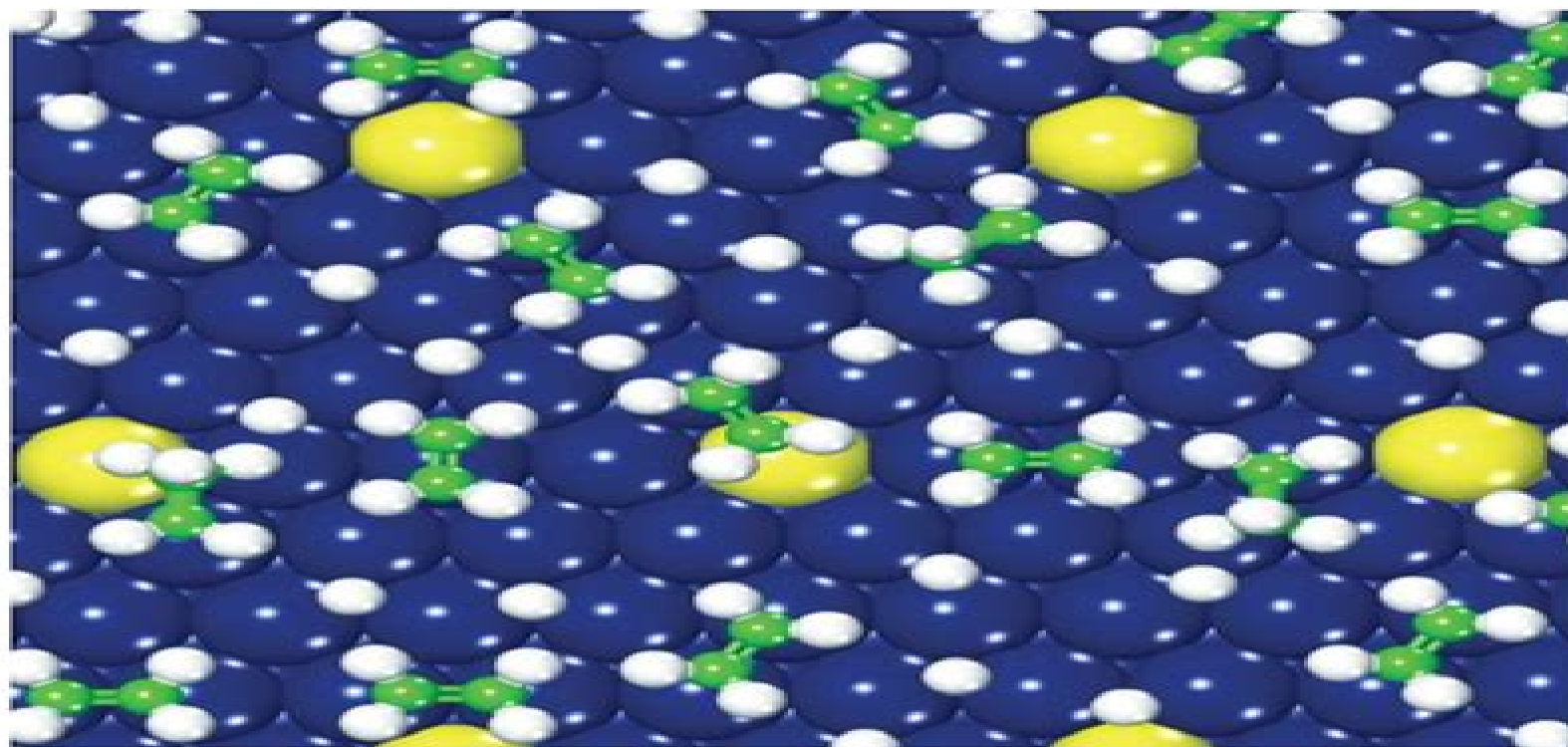


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Molecular Heterogeneous Catalysis

A Conceptual and Computational Approach



Molecular Heterogeneous Catalysis A Conceptual And Computational Approach

Nimir O. Elbashir, Mahmoud M. El-Halwagi, Ioannis G. Economou, Kenneth R. Hall

Molecular Heterogeneous Catalysis A Conceptual And Computational Approach:

Molecular Heterogeneous Catalysis Rutger A. van Santen, Matthew Neurock, 2009-06-10 An integrated approach to the molecular theory of reaction mechanism in heterogeneous catalysis largely based on the knowledge among the growing theoretical catalysis community over the past half century and covering all major catalytic systems The authors develop a general conceptual framework including in depth comparisons with enzyme catalysis biomineralisation organometallic and coordination chemistry A chapter dedicated to molecular electrocatalysis addresses the molecular description of reactions at the liquid solid interphase while studies range from a quantum chemical treatment of individual molecular states to dynamic Monte Carlo simulations including the full flexibility of the many particle systems Complexity in catalysis is explained in chapters on self organization and self assembly of catalysts and other sections are devoted to evolutionary combinatorial techniques as well as artificial chemistry

In-situ Characterization of Heterogeneous Catalysts José A.

Rodriguez, Jonathan C. Hanson, Peter J. Chupas, 2013-04-17 Helps researchers develop new catalysts for sustainable fuel and chemical production Reviewing the latest developments in the field this book explores the in situ characterization of heterogeneous catalysts enabling readers to take full advantage of the sophisticated techniques used to study heterogeneous catalysts and reaction mechanisms In using these techniques readers can learn to improve the selectivity and the performance of catalysts and how to prepare catalysts as efficiently as possible with minimum waste In situ Characterization of Heterogeneous Catalysts features contributions from leading experts in the field of catalysis It begins with an introduction to the fundamentals and then covers Characterization of electronic and structural properties of catalysts using X ray absorption fine structure spectroscopy Techniques for structural characterization based on X ray diffraction neutron scattering and pair distribution function analysis Microscopy and morphological studies Techniques for studying the interaction of adsorbates with catalyst surfaces including infrared spectroscopy Raman spectroscopy EPR and moderate pressure XPS Integration of techniques that provide information on the structural properties of catalysts with techniques that facilitate the study of surface reactions Throughout the book detailed examples illustrate how techniques for studying catalysts and reaction mechanisms can be applied to solve a broad range of problems in heterogeneous catalysis Detailed figures help readers better understand how and why the techniques discussed in the book work At the end of each chapter an extensive set of references leads to the primary literature in the field By explaining step by step modern techniques for the in situ characterization of heterogeneous catalysts this book enables chemical scientists and engineers to better understand catalyst behavior and design new catalysts for green sustainable fuel and chemical production

Design of Heterogeneous Catalysts Umit S. Ozkan, 2009-02-11

This long awaited reference source is the first book to focus on this important and hot topic As such it provides examples from a wide array of fields where catalyst design has been based on new insights and understanding presenting such modern and important topics as self assembly nature inspired catalysis nano scale architecture of surfaces and theoretical methods With

its inclusion of all the useful and powerful tools for the rational design of catalysts this is a true must have book for every researcher in the field *Principles and Practice of Heterogeneous Catalysis* John Meurig Thomas,W. John Thomas,2015-02-09 This long awaited second edition of the successful introduction to the fundamentals of heterogeneous catalysis is now completely revised and updated Written by internationally acclaimed experts this textbook includes fundamentals of adsorption characterizing catalysts and their surfaces the significance of pore structure and surface area solid state and surface chemistry poisoning promotion deactivation and selectivity of catalysts as well as catalytic process engineering A final section provides a number of examples and case histories With its color and numerous graphics plus references to help readers to easily find further reading this is a pivotal work for an understanding of the principles involved

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Natural Gas Processing from Midstream to Downstream provides a broad overview of the current status and challenges for natural gas production treatment and monetization technologies Catalysis Gadi Rothenberg,2017-09-06 This introductory textbook covers all aspects of catalysis It also bridges computational methods industrial applications and green chemistry with over 600 references The book is aimed at chemistry and chemical engineering students and is suitable for both senior undergraduate and graduate level courses with many examples and hands on exercises The author a renowned researcher in catalysis is well known for his clear teaching and writing style he was voted lecturer of the year by the chemistry students Following an introduction to green chemistry and the basics of catalysis the book covers the principles and applications of homogeneous catalysis heterogeneous catalysis and biocatalysis Each chapter includes up to date industrial examples that demonstrate how catalysis helps our society reach the goals of sustainable development Since its publication in 2008 *Catalysis Concepts and Green Applications* has become the most popular textbook in catalysis This second edition is updated with the latest developments in catalysis research in academia and industry It also contains 50 additional exercises based on the suggestions of students and teachers of chemistry and chemical engineering from all over the world The book is also available in the Chinese language <https://detail.tmall.com/item.htm?spm=a212k0.12153887.0.0.4e60687dUTEDKm&id=619581126247> Additional teaching material original figures as PowerPoint lecture slides is freely available in the Supplementary Material

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