

1. Record Nr.	UNINA9910971930403321
Autore	Thomas J. M (John Meurig)
Titolo	Principles and Practice of Heterogeneous Catalysis
Pubbl/distr/stampa	Weinheim : , : John Wiley & Sons, Incorporated, , 2015 ©2015
ISBN	9783527683789 9783527314584
Edizione	[2nd ed.]
Descrizione fisica	1 online resource (769 pages)
Altri autori (Persone)	ThomasW. John
Disciplina	541.3/95
Soggetti	Catalysis Heterogeneous catalysis Science
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Nota di contenuto	Intro -- Principles and Practice of Heterogeneous Catalysis -- Contents -- Preface -- Chapter 1 Setting the Scene -- 1.1 Prologue: Advances since the Early 1990s -- 1.2 Introduction -- 1.2.1 Selectivity of Catalysts -- 1.3 Perspectives in Catalysis: Past, Present and Future -- 1.3.1 Applied Catalysis since the 1940s -- 1.3.2 Some Current Trends in Applied Catalysis -- 1.3.2.1 Auto-Exhaust Catalysts -- 1.3.2.2 Catalysts in Electrochemistry and Photoelectrochemistry -- 1.3.2.3 Immobilized Metals -- 1.3.2.4 Immobilized Enzymes and Cells: Present and Future -- 1.3.2.5 Ribozymes -- 1.4 Definition of Catalytic Activity -- 1.4.1 Magnitude of Turnover Frequencies and Active Site Concentrations -- 1.4.2 Volcano Plots -- 1.4.3 Evolution of Important Concepts and Techniques in Heterogeneous Catalysis -- 1.4.3.1 Mechanistic Insights from Isotopic Labelling -- 1.4.3.2 Concepts from Organometallic Chemistry -- 1.5 Key Advances in Recent Theoretical Treatments: Universability in Heterogeneous Catalysis -- 1.5.1 Some Major Current Developments in Heterogeneous Catalysis -- 1.6 Milestones Reached in Industrial Catalysis in the Twentieth Century, and Some Consequential Challenges -- Problems -- References -- Further Reading -- Chapter 2 The Fundamentals of Adsorption: Structural and Dynamical Considerations, Isotherms and Energetics --

2.1 Catalysis Must Always Be Preceded by Adsorption -- 2.1.1 Physical Adsorption, Chemisorption and Precursor States -- 2.2 The Surfaces of Clean Solids are Sometimes Reconstructed -- 2.3 There Are Many Well-Defined Kinds of Ordered Adlayers -- 2.4 Adsorption Isotherms and Isobars -- 2.4.1 The Empirical Facts -- 2.4.2 Information That Can Be Gleaned from Isotherms -- 2.4.3 Adsorption Is Almost Invariably Exothermic -- 2.5 Dynamical Considerations -- 2.5.1 Residence Times -- 2.5.2 Rates of Adsorption.
2.5.3 Applying Statistical Mechanics to Adsorption -- 2.5.4 Adsorption Kinetics Can Often Be Represented by the Elovich Equation -- 2.5.5 Rates of Desorption -- 2.5.6 Applying Statistical Mechanics to Desorption -- 2.5.7 Influence of a Precursor State on the Kinetics of Desorption -- 2.6 Relating the Activation Energy to the Energy of Chemisorption. Universality in Heterogeneous Catalysis and the Brønsted-Evans-Polanyi (BEP) Relation -- 2.6.1 Pareto-Optimal Catalysts -- 2.7 Deriving Adsorption Isotherms from Kinetic Principles -- 2.7.1 Using the Langmuir Isotherm to Estimate the Proportions of Non-dissociative and Associative Adsorption -- 2.7.2 Other Adsorption Isotherms -- 2.7.2.1 Henry's Adsorption Isotherm -- 2.7.2.2 Freundlich Isotherm -- 2.7.2.3 Temkin Isotherm -- 2.7.2.4 Brunauer-Emmett-Teller Isotherm -- 2.7.2.5 Developments from Polanyi's Adsorption Theory -- 2.7.2.6 Kaganer's Isotherm and the DKR Equation -- 2.7.2.7 Virial Equation of State -- 2.8 Energetics of Adsorption -- 2.8.1 Estimating the Binding Energies of Physically Adsorbed Species -- 2.8.2 Binding Energies of Chemisorbed Species -- 2.8.3 Estimating Heats of Adsorption from Thermodynamic Data -- 2.8.4 Decline of the Heat of Adsorption with Increasing Coverage -- 2.9 Mobility at Surfaces -- 2.10 Kinetics of Surface Reactions -- 2.10.1 The Influences of Precursor States on the Kinetics and Energy Distribution of Catalysed Reactions -- 2.10.2 Comparing the Rates of Heterogeneous and Homogeneous Reactions -- 2.11 Autocatalytic, Oscillatory and Complex Heterogeneous Reactions -- 2.11.1 An Outline of Autocatalysis -- 2.11.2 Background to Oscillating Reactions -- 2.11.3 Instabilities and Transient Phenomena in Heterogeneous Catalysis -- 2.11.4 Multiple Steady States -- 2.11.5 Transient Phenomena -- 2.11.6 Recent Thoughts on Spatio-Temporal Behaviour and Turbulence at Catalyst Surfaces.
2.12 Microkinetics: A Summary -- 2.12.1 Building Kinetic Models -- 2.12.2 Formulation of Kinetic Models in Terms of Transition States -- 2.12.3 Degree of Rate Control -- Problems -- References -- Further Reading -- Chapter 3 The Characterization of Industrial and Model Solid Catalysts -- Part I: Characterization of Industrial Solid Catalysts -- 3.1 Non-invasive Methods Suitable for Studies Involving Catalytic Reactors -- 3.1.1 Magnetic Resonance Imaging (MRI) -- 3.1.1.1 Visualizing the Spatial Variation of Esterification, Etherification and Hydrogenation within Fixed-Bed and Trickle-Bed Reactors with MRI -- 3.1.2 Positron Emission Methods -- 3.1.3 Use of Spatially-Resolved X-ray Absorption to Probe Supported Nobel Metal Catalysts during Operating Conditions -- Part II: Laboratory Characterization of Solid Catalysts -- 3.2 A Portfolio of Modern Methods: Introducing the Acronyms -- 3.3 Which Elements and Which Phases Are Present? -- 3.3.1 X-ray Fluorescence (XRF), X-ray Emission (XRE) and Proton-Induced X-ray Emission (PIXE) -- 3.3.2 Developing Techniques: ICPMS -- 3.3.3 X-ray Diffraction (XRD) and Small-Angle X-ray Scattering -- 3.3.3.1 Mean Size, Surface Area and Particle-Size Distribution from SAXS -- 3.3.3.2 In situ Studies by X-ray Diffraction -- 3.3.3.3 Experimental Aspects -- 3.4 Probing Surfaces with IR, HREELS, AES and XPS -- 3.4.1 Infrared Spectroscopy (IR): A Non-destructive Technique

Usable on Catalysts Exposed to High Pressure -- 3.4.2 High-Resolution Electron-Energy Loss Spectroscopy (HREELS): the Most Sensitive Tool for Identifying Surface Vibrational Modes -- 3.4.3 Merits and Limitations of Electron Spectroscopy -- 3.5 Ultraviolet-Visible and Photoluminescence Spectroscopy -- 3.6 Structure and Crystallography of Surfaces: Nature of Ordered and Reconstructed Surfaces -- 3.6.1 Two- and Three-Dimensional Surface Crystallography.
3.6.2 Notations for Describing Ordered Structures at Surfaces -- 3.6.3 How Do Bond Distances at Surfaces Compare with Those of Bulk Solids? What of Displacive Reconstructions? -- 3.6.4 EXAFS, SEXAFS, XANES and NEXAFS: Probing Bond Distances and Site Environments Even When There is No Long-Range Order -- 3.6.4.1 Origin of EXAFS and How It Is Used -- 3.6.4.2 Applications of EXAFS to the Study of Catalysts -- 3.6.4.3 SEXAFS -- 3.6.4.4 XANES and Pre-edge Structure: Deducing Site Symmetry and Oxidation States -- 3.6.4.5 NEXAFS -- 3.7 Other Structural Techniques for Characterizing Bulk and Surfaces of Catalysts -- 3.7.1 Electron Spin Resonance (ESR): Probing the Nature of Catalytically Active Sites and the Concentration of Paramagnetic Intermediates on Surfaces and in the Gas Phase -- 3.7.1.1 Examples of the Use of ESR in Heterogeneous Catalysis -- 3.7.2 Nuclear Magnetic Resonance (NMR): A Technique Applicable, at High Resolution, to Solids and Their Surfaces -- 3.7.2.1 Basic Principles -- 3.7.2.2 NMR Spectra of Solids -- 3.7.2.3 Applications of NMR to the Study of Catalysts, Adsorbents and Adsorbates -- 3.7.2.4 Future Prospects for the Study of Catalysts by Solid-State NMR -- 3.7.3 Sum Frequency Generation (SFG) and Infrared Reflection Absorption Spectroscopy (IRAS or IRRAS) -- 3.7.3.1 Essential Background and Mode of Operation -- 3.7.4 Scanning Tunnelling Microscopy (STM) and Clues for the Design of New Catalysts -- 3.7.4.1 Scanning Tunnelling Spectroscopy (STS) -- 3.7.4.2 Atomic Force Microscopy (AFM) and Fluorescence Microscopy (FM) -- 3.7.5 Electron Microscopy -- 3.7.5.1 Electron Crystallography -- 3.7.5.2 Electron Tomography (ET) -- 3.7.5.3 A Few Illustrative Examples of Static EM Images -- 3.7.5.4 In situ (Environmental) TEM -- 3.7.5.5 4D Electron Microscopy -- 3.7.6 Optical Microscopy and Ellipsometry (Non-invasive Techniques).
3.7.7 Neutron Scattering: A Technique of Growing Importance in the Study of Catalysts -- 3.7.7.1 Determining the Atomic Structure and Texture of Microcrystalline Catalysts, the Nature of the Active Sites and the Disposition of Bound Reactants -- 3.7.7.2 Determining the Structure of, and Identifying Functional Groups in, Chemisorbed Layers at Catalyst Surfaces -- 3.8 A Miscellany of Other Procedures -- 3.9 Determining the Strength of Surface Bonds: Thermal and Other Temperature-Programmed Methods -- 3.9.1 Temperature-Programmed Desorption (TPD) or Flash Desorption Spectroscopy (FDS) -- 3.9.2 Temperature-Programmed Reaction Spectroscopy (TPRS) -- 3.9.3 Magnitude of the Heat and Entropy of Adsorption -- 3.10 Reflections on the Current Scene Pertaining In situ Methods of Studying Catalysts -- 3.10.1 Isotopic Labelling and Transient Response -- 3.10.2 From Temporal Analysis of Products (TAP) to Steady-State Isotopic Transient Kinetic Analysis (SSITKA) -- 3.10.3 Infrared, Raman, NMR, and X-ray Absorption Spectroscopy for In situ Studies -- 3.10.4 In situ X-ray, Electron and Neutron Diffraction Studies -- 3.10.5 Combined X-ray Absorption and X-ray Diffraction and Other Techniques for In situ Studies of Catalysts -- Problems -- References -- Further Reading -- General -- Additional -- In situ Techniques -- Chapter 4 Porous Catalysts: Their Nature and Importance -- 4.1 Definitions and Introduction -- 4.2 Determination of Surface Area -- 4.2.1 Assessment of Porosity -- 4.2.1.1 Capillary Condensation -- the

Kelvin Equation and the Barrett-Joyner-Halenda Method -- 4.2.2
Evaluation of Both Micropore and Mesopore Size Using Density Functional Theory and Grand Canonical Monte Carlo Methods --
4.2.2.1 An Explanatory Note about Density Functional Theory (DFT) in the Context of Adsorption -- 4.2.2.2 How Does One Tackle a 'Breathing' MOF Nanoporous Structure?.
4.2.3 The Fractal Approach.

Sommario/riassunto

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.
