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and in order to
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develop catalyst
design strategies, an
identification of key
parameters, that are
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for the catalytic rate

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and selectivity
(lumped together as
"activity" in the
following) is needed.

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catalysis with its
simple operation and
industrial compatibility
can be an effective
means of achieving

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this challenging task.

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carbon monoxide,
alcohols, and
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Modeling
In industry, many
design variables must
be considered
including reactor and
catalyst design across
multiple scales

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ranging from the
subnanometer to tens
of meters. The
conventional

heterogeneous
catalysis reactors
include batch ,
continuous , and
fluidized-bed reactors
, while more recent
setups include fixed-
bed, microchannel,
and multi-functional
reactors . [7]

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The project is entitled

“Design of

heterogeneous

catalysts”. Three

selected reactions

have been

investigated in detail

during the studies,

namely the

methanation reaction,

the Fischer- Tropsch

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process, and the ammonia-based selective catalytic reduction (SCR).

These reactions will be described in three separate parts.

Design of heterogeneous catalysts

In this regard, metal-organic frameworks (MOFs)

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offer great
opportunities for the
rational design of new
catalytic solids, as

highlighted by the
unprecedented
number of
publications

appearing over the
past decade. In this
review, the recent
advances in the
application of MOFs
in heterogeneous

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catalysis are
discussed.

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Metal–Organic
Frameworks in
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Catalysis ...

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Modeling
It has recently been
demonstrated that the
dynamic behaviour of
surface-supported
nanocluster catalysts
in realistic reaction
conditions defies

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conventional models used in catalysis. This opens new doors in catalysis by giving more leverage in catalyst design, but also requires a major revision of the understanding of how dynamic heterogeneous catalytic interfaces operate, as well as of the computational

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catalysts obtained by
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mesoporous silica;
Design, synthesis and
in situ

characterisation of
new solid catalysts

(Linus Pauling
Lecture, California
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Lecture, Max Planck
Institute, Mülheim,
November 1998.)

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John Meurig Thomas
- Wikipedia

In a recent study
published in ACS

Catalysis, a team of
scientists from Tokyo
Tech, Japan, came up
with a new idea for a
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catalyst. They chose
nanoporous zirconium
carbide (ZrC) as the...

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This long-awaited

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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-

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nano-scale
architecture of
surfaces and
theoretical methods.

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the useful and
powerful tools for the
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Presents state-of-the-art knowledge of heterogeneous catalysts new approaches including new applications in energy and environmental fields

This book focuses on emerging techniques in heterogeneous catalysis, from new methodology for catalysts design and synthesis, surface

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with an overview on

the evolution in

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precise understanding
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catalysts play an

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of today's processes

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emphasis on

sustainability in both
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processes, this

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topics of heterogeneous catalysis and clean technology. It focuses on the development of heterogeneous catalysts for use in clean chemical synthesis, dealing with how modern spectroscopic techniques can aid the design of catalysts for use in liquid phase

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heterogeneous reactions, their application in industrially important chemistries - including selective oxidation, hydrogenation, solid acid- and base-catalyzed processes - as well as the role of process intensification and use of renewable resources in improving the sustainability of

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chemical processes.
With its emphasis on
applications, this book
is of high interest to
those working in the
industry.

For far too long
chemists and
industrialists have
relied on the use of
aggressive reagents
such as nitric and
sulphuric acids,

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permanganates and dichromates to prepare the massive quantities of both bulk and fine chemicals that are needed for the maintenance of civilised life □

materials such as fuels, fabrics, foodstuffs, fertilisers and pharmaceuticals. Such aggressive reagents generate

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vast quantities of environmentally harmful and often toxic by-products, including the oxides of nitrogen, of metal oxides and carbon dioxide. Now, owing to recent advances made in the synthesis of nanoporous solids, it is feasible to design new solid catalysts that enable benign,

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mild oxidants to be used, frequently without utilising solvents, to manufacture the products that the chemical, pharmaceutical, agro- and bio-chemical industries require. These new solid agents are designated single-site heterogeneous

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catalysts (SSHCs).

Their principal characteristics are that all the active sites present in the high-area solids are identical in their atomic environment and hence in their energy of interaction with reactants, just as in enzymes. Single-site heterogeneous catalysts now occupy

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a position of growing
importance both
academically and in
their potential for
commercial

exploitation. This text,
the only one devoted
to such catalysts,
dwells both on

principles of design
and on applications,
such as the benign
synthesis of nylon 6
and vitamin B3. It

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Equips the reader with unifying insights required for future catalytic adventures in the quest for sustainability in the materials used by humankind. Anyone acquainted with the language of molecules, including undergraduates in the physical and biological sciences,

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as well as graduates in engineering and materials science, should be able to assimilate the principles and examples presented in this book. Inter alia, it describes how clean technology and "green" processes may be carried out in an environmentally responsible manner.

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design principles

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energy transformation
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several semesters

Heterogeneous
catalysis plays a part
in the production of
more than 80% of all
chemical products. It
is therefore essential

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that all chemists and
chemical engineers
have an

understanding of the
fundamental

principles as well as
the applications of
heterogeneous

catalysts. This book
introduces the

subject, starting at a
basic level, and

includes sections on
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surface science, heterogeneous catalytic kinetics, experimental methods for preparing and studying heterogeneous catalysts, as well as some aspects of the design of industrial catalytic reactors. It ends with a chapter that covers a range of examples of important catalytic processes.

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The book leads the student to carrying out a series of "tasks" based on searches of the internet and also on the use of web-based search tools such as Scopus or Web of Science.

These tasks are generally based on the text; they can be used entirely for self-study but they can

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also be tailored to the requirements of a particular course by the instructor/lecturer giving the course. The author has had over 40 years of experience in catalytic research as well as in lecturing on the principles of catalysis. He was for more than 20 years the Editor of Catalysis Today.

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aspects of catalysis in
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text Inclusion of

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historical
development of the
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personalities involved
All concepts

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Heterogeneous

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catalysis plays a central role in the global energy paradigm, with practically all energy-related process relying on a catalyst at a certain point. The application of heterogeneous catalysts will be of paramount importance to achieve the transition towards

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low carbon and sustainable societies. This book provides an overview of the design, limitations and challenges of heterogeneous catalysts for energy applications. In an attempt to cover a broad spectrum of scenarios, the book considers traditional processes linked to

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fossil fuels such as
reforming and
hydrocracking, as well
as catalysis for

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CO₂ to clean fuels.

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catalysis has
undergone a
revolutionary change
in the past two
decades due to the

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characterization
methods that provide
fundamental
information about the
catalyst bulk
structures, surfaces,
and their properties.
For the first time,
these characterization
methods have
allowed researchers
to "see" the surfaces

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of catalytic materials, their bulk structures (crystalline as well as amorphous phases), the influence of the process conditions on the catalytic material, as well as the effect of different synthesis methods. This new information has tremendously advanced our understanding of

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their properties.

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methods have
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and are indispensable
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materials. It is hard to
conceive of a modern
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