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Reactivity
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Reactivity
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Volume 3 of the
5-volume
Quantum
Nanochemistry
presents the

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chemical
reactivity
throughout the
molecular
structure in
general and
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bonding in
particular by
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quantum bosonic
particles of

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from Huckel to
Density
Functional
expositions,
especially in
relation to how
chemical princi
Drawn from
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sources, this

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book provides principles and strategies for the evaluation of chemical reactions, and for using this information in process design and management. A useful resource for engineers who

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design, start-up, operate, and manage chemical and petrochemical plants, the book places special emphasis on the use of state-of-the-art technology in theory, testing

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methods, and
Reactivity
applications in
International
design and
Edition
operations.

Kotz/Treichel/W
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Reactivity,
Sixth Enhanced
Review Edition
includes unique
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sections that are designed to help students prepare for multiple chapter exams. These new sections provide additional questions, including molecular and

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applied
problems,
linked to
chapter goals
and
corresponding
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softbound and
less expensive
than the

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version.

Discusses
chemical
reactions,
examining the
bonding in
molecules, how
molecules
interact, what
determines
whether an
interaction is
favourable or

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not, and what
the outcome
will be.

Conformation,
Configuration,
Stereoelectroni
c Effects and
Asymmetric
Synthesis
Student
Solutions
Manual for Use
with Chemistry

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A Density
Reactivity
Functional View
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Chemical
Editions
Principles
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of Numerical
Data, Physics,
Chemistry and
Technology
School Version
With General
Chemistrynow

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**Taking an evidence-
first big picture
approach,**

**Chemistry: Human
Activity, Chemical
Reactivity**

**encourages
students to think
like a chemist,
develop critical
understanding of
what chemistry is,
why it is important
and how chemists**

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And Chemical
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**arrive at their
discoveries.**

**Flipping the
traditional model
of presenting facts
and building to
applications, this
text begins with
contexts that are
real-life and
matter to students
- from doping in
sports, to the
chemistry behind**

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**the treads of wall-
climbing robots.**

**Informed by the
latest chemical
education**

research,

**Chemistry: Human
Activity, Chemical
Reactivity presents
chemistry as the
exciting,**

**developing human
activity that it is,
rather than a body**

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of facts, theories,

and skills handed

down from the

past. Along with

the innovative

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and OWLv2

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unique case

studies and

critically acclaimed

interactive e-

resources to help

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chemistry and how**

it is helping to

address global

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In the 1970s,

Density Functional

Theory (DFT) was

borrowed from

physics and

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**adapted to
chemistry by a
handful of
visionaries. Now
chemical DFT is a
diverse and rapidly
growing field, its
progress fueled by
numerous
developing
practical
descriptors that
make DFT as
useful as it is vast.**

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from 13 different

countries,

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Reactivity Theory:

A Density

Functional View

represents the

true collaborative

spirit and

excitement of

purpose

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Electron

engendered by the study and use of DFT. This work instructs readers on how concepts from DFT can be used to describe, understand, and predict chemical reactivity. Prior knowledge is not required as early chapters, written by the field's

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state DFT and its

extensions to time-

dependent

systems, excited

states, and spin-

polarized

molecules. While

the text is

accessible to

senior

undergraduate or

beginning

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**graduate students,
experienced**

researchers are

certain to find

interesting new

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perspectives

presented by these

seasoned experts.

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resource—

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authoritative

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**accounts on
aspects of the
theory of chemical
reactivity**

**Describes various
global reactivity
descriptors, such
as**

**electronegativity,
hardness, and
electrophilicity**

**Introduces and
analyzes the
usefulness of local**

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reactivity

descriptors such as

Fukui, shape, and

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localization

functions Offers an

in-depth analysis

of how chemical

reactivity changes

during different

physicochemical

processes or in the

presence of

external

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**perturbations The
book covers a**

gamut of related

topics such as

methods for

determining atoms-

in-molecules,

population

analysis,

electrostatic

potential,

molecular quantum

similarity,

aromaticity, and

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biological activity.
It also discusses

the role of

reactivity concepts

in industrial and

other practical

applications.

Whether you are

searching for new

products or new

research projects,

this is the ultimate

guide for

understanding

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reactivity.**

**Provides an
account of the
fundamental
principles of the
density-functional
theory of the
electronic
structure of matter
and its
applications to
atoms and
molecules. This**

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**book contains a
discussion of the
chemical potential
and its derivatives.
It is intended for
physicists,
chemists, and
advanced students
in chemistry.**

**Stereochemistry
and Organic
Reactions
From Molecular
Structure to**

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Insight**

**Tutorials in
Molecular Reaction
Dynamics**

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Catalysis:**

**Proceedings of a
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A decade ago,

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the U.S.
chemical
industry was
in decline. Of
the more than
40 chemical
manufacturing
plants being
built
worldwide in
the mid-2000s
with more than

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\$1 billion in
capitalization

, none were

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construction

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States. Today,

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affordable

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natural gas
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resulting from
the dramatic
rise in shale
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gas liquids
provides an
opportunity to
discover and
develop new
catalysts and
processes to
enable the
direct
conversion of
natural gas
and natural

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gas liquids
into value-
added
chemicals with
a lower carbon
footprint. The
economic
implications
of developing
advanced
technologies
to utilize and

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process
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natural gas
International
Edition
and natural
gas liquids

for chemical
production
could be
significant,
as commodity,
intermediate,
and fine
chemicals

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represent a higher-economic-value use of shale gas

compared with its use as a fuel. To

better

understand the opportunities for catalysis research in an

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era of
shifting
feedstocks for
chemical
production and
to identify
the gaps in
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research
portfolio, the
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Academies of

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Sciences,
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Engineering,
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conducted an
interactive, m
ultidisciplina
ry workshop in
March 2016.
The goal of
this workshop
was to
identify

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advances in
catalysis that
can enable the
United States
to fully
realize the
potential of
the shale gas
revolution for
the U.S.
chemical
industry and,

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as a result,
to help target
the efforts of
U.S.

researchers
and funding
agencies on
those areas of
science and
technology
development
that are most

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critical to
achieving
these
advances. This
publication
summarizes the
presentations
and
discussions
from the
workshop.
The text opens

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with an
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overview of
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the way
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chemists
understand
chemical
structure. The
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the text
presents a
mechanistic
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of modern
organic
chemistry,
developed in
the context of
synthetic
organic
chemistry and
exemplified by
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analysis of
confined
chemical
systems for
theoretical
and
experimental
scientists

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Systems:

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presents a
theoretical
basis for the
molecular
phenomena
observed in

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confined
spaces. The
book
highlights sta
te-of-the-art
theoretical
and
computational
approaches,
with a focus
on obtaining
physically

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clarification
of the subject
to enable the
reader to
build an
appreciation
of underlying
chemical
principles.

The book
includes real-

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world examples

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of confined

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systems that

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highlight how

the reactivity

of atoms and

molecules

change upon

encapsulation.

Chapters

include

discussions on

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recent

developments

related to

several host-

guest systems,

including cucu

rbit[n]uril,

ExBox+4,

clathrate

hydrates, octa

acid cavitand,

metal organic

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frameworks
(MOFs),
covalent
organic
frameworks
(COFs),
zeolites,
fullerenes,
and carbon
nanotubes.
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learn how to

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carry out new
calculations
to understand
the physicoche
mical behavior
of confined
quantum
systems.

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thorough
introduction

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to global
reactivity
descriptors,
including elec
tronegativity,
hardness, and
electrophilici
ty An
exploration of
the Fukui
function, as
well as dual

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reactivity and

temperature

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localization
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the solvent

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and
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chemistry and
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working in the
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catalysis,

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chemistry, and

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materials.

Over the past

25 years, the

molecular

electrostatic

potential has

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become firmly
established as
an effective
guide to
molecular
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With the
recent
advances in
computational
technology, it
is currently

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being applied
to a variety
of important
chemical and
biological
systems. Its
range of
applicability
has expanded
from primarily
a focus on
sites for

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electrophilic
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attack to now

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effects,

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zeolite,

molecular

cluster and

crystal

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behavior, and
the

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correlation

and prediction

of a wide

range of

macroscopic

properties.

Moreover, the

increasing

prominence of

density

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functional
theory has
raised the
molecular
electrostatic
potential to a
new stature on
a more
fundamental
conceptual
level. It is
rigorously

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defined in
terms of the
electron
density, and
has very
interesting
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since it
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opposing

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nuclei and the
electrons.

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opens with a
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by one of the
original
pioneers of
the use of the
electrostatic

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potential in
studies of

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chemical

reactivity,

Jacopo Tomasi.

Though the

flow of the

succeeding

chapters is

not

stringently

defined, the

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overall trend
is that the
emphasis
changes
gradually from
methodology to
applications.
Chapters
discussing
more
theoretical
topics are

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find the wide
variety of
topics
provided by an
international
group of
authors both
convincing and
useful.

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Atoms and
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Guidelines for
Process Safety
in Batch

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Adhesives are widely used in the manufacture and assembly of electronic circuits and products. Generally, electronics design engineers and manufacturing engineers are not well versed in adhesives,

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while adhesion chemists have a limited knowledge of electronics. This book bridges these knowledge gaps and is useful to both groups. The book includes chapters covering types of adhesive, the chemistry on which they are based, and their properties,

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*applications,
processes,
specifications, and
reliability. Coverage
of toxicity,
environmental impacts
and the regulatory
framework make this
book particularly
important for
engineers and
managers alike. The
third edition has been*

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*updated throughout
and includes new
sections on
nanomaterials,
environmental impacts
and new
environmentally
friendly 'green'
adhesives.*

*Information about
regulations and
compliance has been
brought fully up-to-*

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date. As well as providing full coverage of standard adhesive types, Licari explores the most recent developments in fields such as:

- *Tamper-proof adhesives for electronic security devices.*
- *Bio-compatible adhesives for implantable*

medical devices. •

*Electrically
conductive adhesives
to replace toxic tin-
lead solders in printed
circuit assembly – as
required by regulatory
regimes, e.g. the EU's
Restriction of
Hazardous Substances
Directive or RoHS
(compliance is
required for all*

products placed on the European market). • Nano-fillers in adhesives, used to increase the thermal conductivity of current adhesives for cooling electronic devices. A complete guide for the electronics industry to adhesive types, their properties and applications – this

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*book is an essential
reference for a wide
range of specialists
including electrical
engineers, adhesion
chemists and other
engineering
professionals Provides
specifications of
adhesives for
particular uses and
outlines the processes
for application and*

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curing – coverage that is of particular benefit to design engineers, who are charged with creating the interface between the adhesive material and the microelectronic device
Discusses the respective advantages and limitations of different adhesives for a varying

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*applications, thereby
addressing reliability
issues before they
occur and offering
useful information to
both design engineers
and Quality*

*Assurance personnel
Stereochemistry and
Organic Reactions:
Conformation,
Configuration,
Stereoelectronic*

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*Effects and
Asymmetric Synthesis
provides coverage on
the stereochemistry of
reactions of all
mechanistic types,
ranging from ionic,
pericyclic and
transition metal-
catalyzed to radical
and photochemical.
Chapters cover
acyclic molecules,*

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cyclic molecules, the stereochemistry of organic reactions, the perturbation molecular orbital theory for the origin of stereoelectronic effects, and an introduction to the principles of stereoselectivity and hierarchical levels of asymmetric synthesis.

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Each chapter includes problems that reinforce main themes, making it valuable to students, teachers and researchers working in organic, biological and medicinal chemistry, as well as biologists, pharmacologists, polymer chemists and

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chemists. Presents a holistic and unified approach to stereochemical understanding and predictions, covering reactions of all mechanistic classes Includes two background chapters on perturbation theory and stereoselective principles, along with

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*asymmetric designs
Features novel rules
and mnemonics to
delineate product
stereochemistry
Includes up-to-date
coverage with over
1300 selective
references
Emphasises on
contemporary
applications and an
intuitive problem-*

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solving approach that helps students discover the exciting potential of chemical science. This book incorporates fresh applications from the three major areas of modern research: materials, environmental chemistry, and biological science.

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with the clear
explanations, problem-
solving strategies, and
dynamic study tools of
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CHEMICAL
REACTIVITY, 9e.*

*Combining thorough
instruction with the
powerful multimedia
tools you need to
develop a deeper*

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*understanding of
general chemistry
concepts, the text
emphasizes the visual
nature of chemistry,
illustrating the close
interrelationship of
the macroscopic,
symbolic, and
particulate levels of
chemistry. The art
program illustrates
each of these levels in*

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and Organic*

Chemical Reactions

Chemistry

Frontier Orbitals and

Reaction Paths

Connections to Our

Changing World

Chemical Kinetics

Chemistry of Silica

and Zeolite-Based

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instruction with
powerful
multimedia tools
to give you a
deeper**

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general chemistry**

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signature logical

organization,

macro to micro

orientation, and

superior art

program with new

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better prepare for**

**multiple chapter
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points lists, and

new exam-type

questions for

multiple chapters

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grouped according to where most exams occur in the course. The text emphasizes the visual nature of chemistry and illustrates the interrelationship of the macroscopic, symbolic, and

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of chemistry.**

With clear

writing, seamless

technology

integration, and

robust homework

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tools, the text

equips you with

tools to empower

the mastery,

assignment, and

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**assessment of
chemical
principles. The
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reveals these
three levels in
engaging detail-
and is fully
integrated with
new key media
components. The
Web-based
tutorial**

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meet your
specific needs,
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clips, and more,

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REACTIVITY,
INTERNATIONAL
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completely
integrated with
accompanying
technology than
any other text on
the market.

**CHEMISTRY AND
CHEMICAL
REACTIVITY** has

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been revised to help students get to a higher level of understanding of General Chemistry-concepts.

This revision includes General ChemistryNow, a new CD-ROM and web-based learning system that focuses on

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**goals,
connections, and
complete
integration with
the text.**

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calculus-inclusive
general chemistry
courses,
Chemical
Principles helps
students develop
chemical insight**

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by showing the connections between fundamental chemical ideas and their applications. Unlike other texts, it begins with a detailed picture of the atom then builds toward

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**chemistry's
frontier,
continually
demonstrating
how to solve
problems, think
about nature and
matter, and
visualize
chemical
concepts as
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do. Flexibility in**

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**level is crucial,
and is largely
established
through clearly
labeling
(separating in
boxes) the
calculus coverage
in the text:
Instructors have
the option of
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incorporate**

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students can take
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showing how
organic,
inorganic, and
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can be blended
together to**

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**The Changing
Landscape of
Hydrocarbon
Feedstocks for
Chemical
Production
Selected Papers
of Kenichi Fukui
Structure and
Reactivity in
Organic
Chemistry
Quantum**

Page 111/199

And Chemical
**Molecules and
Reactivity**

"Chapter Goals" and
"Chapter Goals
Revisited" are two
new features in this
revision. Each
chapter starts with a
list of goals that
allows students to
see what is ahead.
The chapter
concludes with a
repetition of that list

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with summary
information added.

General

ChemistryNow is correlated to this list. New to this edition are dozens of "Active Figures" to help students visualize chemistry in action. These animated versions of text art help students master key

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concepts from the
book. "Active

Figures" can be

used as

demonstrations in

the classroom and

each figure is paired

with a guided

exploration and

exercise to ensure

students understand

the concept being

illustrated. In-text

worked "Examples"

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follow a four-part structure: "Problem" statement,

"Strategy" for approaching the problem, fully worked "Solution," and, where

appropriate, a "Comment" on the problem and solution. Through this approach, students learn how

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to approach a problem rather than merely learning to memorize problem types and memorized solution approaches.

Exercises appear throughout the text so students can check their comprehension of the material.

Answers are in an

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appendix. "Problem-Solving Tips"

provide readers tips for determining how to approach and solve problems.

"Chemical Perspectives" are essays that bring relevance and perspective to a study of chemistry. In order to put chemistry in its

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historical context,
"Historical

Perspective" essays

describe the people

who were key to

developing the

concepts of the

chapter. "A Closer

Look" essays

describe ideas that

form the

background to

material under

discussion or

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provide another dimension of the subject. - Publisher.

Density Functional Theory (or DFT for short) is a potent methodology useful for calculating and understanding the molecular and electronic structure of atoms, molecules, clusters, and solids. Its use relies not

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only in the ability to
calculate the

molecular properties
of the species of

interest but also
provides interesting
concepts that allow
a better

comprehension of
the chemical
reactivity of the
studied systems.

This book
represents an

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attempt to present

examples on the

utility of DFT for the

understanding of

the chemical

reactivity through

descriptors that

constitute the basis

of the so called

Conceptual DFT

(sometimes also

named as Chemical

Reactivity Theory)

as well as the

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application of the
theory and its

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procedures in the
determination of the
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of different systems
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industrial interest.

Batch reaction
systems pose
unique challenges
to process safety

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managers because they do not operate in a steady state.

The sequence of processing steps, and frequent start-ups and shutdowns, increase the possibility of human errors and equipment failures. And, since batch plants are often designed for shared

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use, frequent
modification of
piping and layout
may occur, resulting
in complex
"management of
change" issues.
This book identifies
the singular
concerns of batch
reaction
systems—including
potential sources of
unsafe

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conditions—and provides a "how-to" guide for the practicing engineer in dealing with them by applying appropriate practices to prevent accidents.

Summarizes core information for quick reference in the workplace, using tables and

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governing the use,
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specialized

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QA Manager at the

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Laboratory at Port

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member of the

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and Health, of the

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Loss Prevention
Reactivity Panel and of the

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'Exposure Limits

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and a consultant. He

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courses of the
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Bulletin, April 1994 -

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many practical

applications.

The formulation

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of the Intrinsic
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Reaction

Coordinate and
Applications to
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systems are also
presented. The
aim of this
volume is to
show by what
forces chemical
reactions are
driven and to
demonstrate how

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the regio- and s
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are determined

in chemical

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investigators

will gain

insight into the

nature of

chemical

reactions and

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find out how
quantum chemical
calculations are
connected with
chemical
intuition.

The principal
theme of this
book is to
provide a broad
overview of the
principles of
chemistry and
the reactivity

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of the chemical
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elements and
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encourages students

to think like a chemist,

develop critical

understanding of what

chemistry is, why it is

important and how

chemists arrive at

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chemist's skills to have
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with molecular orbital
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information can be viewed here. "These books are the result of years of work, which began as an attempt to write a second edition of my 1976 book Frontier Orbitals and Organic Chemical Reactions. I wanted to give a rather more thorough introduction to molecular orbitals,

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while maintaining my focus on the organic chemist who did not want a mathematical account, but still wanted to understand organic chemistry at a physical level. I'm delighted to win this prize, and hope a new generation of chemists will benefit from these books." —Professor

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Kinetics bridges

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transfers and
electron
transfers. For the
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provides the
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experiments, and
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combine to offer
a panorama of
time-dependent
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*phenomena
connected by a
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qualitative
description: with
the guidance of
theory, the path
becomes a
reaction path
that can actually
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**calculated. But
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Kinetics is more

about structure

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than numbers

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mechanisms with

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and how

molecular

structures

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related to silica-
based materials
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different fields of
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Since silica is
transparent and
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it is a very***

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and biological***

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this field seeking
an***

***understanding of
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***applications of
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various fields
using silica
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molecules in
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catalysis and
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and other topics
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