Computer Simulation of Porous Materials
Current Approaches and Future Opportunities

Kim Jelfs Imperial College London, UK

Synopsis

Computer Simulation of Porous Materials covers the key approaches in the modelling of porous materials, with a focus on how these can be used for structure prediction and to either rationalise or predict a range of properties. Through chapters focusing on techniques for specific types of applications and properties, it outlines the challenges and opportunities in applying approaches and methods to different classes of systems, including a discussion of high-throughput screening. Edited by a world leader in the field, this title is presented at a level accessible to advanced undergraduates, postgraduates and researchers wishing to learn more about the topic.

Brief Contents

- Introduction to Computational Modelling of Microporous Materials
- Structure Prediction of Porous Materials
- Atomistic Simulations of Mechanical Properties
- Modelling Sorption and Diffusion Behaviour in Porous Solids
- Spectroscopic and Catalytic Properties
- Machine Learning in Porous Materials
Advance Book Information

Gibbs Energy and Helmholtz Energy
Liquids, Solutions and Vapours

Emmerich Wilhelm
University of Vienna, Austria
Trevor M Letcher
University of KwaZulu-Natal, South Africa

Synopsis
This volume is a comprehensive collection of chapters written by an international team of world authorities and contains the latest information on all aspects of the most important chemical thermodynamic properties of Gibbs energy and Helmholtz energy, as related to fluids. This new book covers the wide range of topics in the field and as such is a key point of reference for advanced undergraduates and graduates alike as well as researchers, academics and anyone working in the field or related areas.

Brief Contents
- Gibbs Energy and Helmholtz Energy: Introduction, Concepts and Selected Applications
- Low-pressure Solubility of Gases in Liquids
- Assembly of Hard Spheres in Liquid Water
- Excess Molar Gibbs Energies: Related Properties and Formalisms Using DISQUAC
- Simultaneous Determination of Equilibrium Constants, Enthalpy Changes and Stoichiometries by Titration Calorimetry
- Solvation Free Energy by 3D-RISM-KH Theory
- Calculation Procedure to Check the Quality of Vapour-Liquid Equilibrium Data
- Correlative and Predictive Models for GE
- Gibbs Energies in Biomolecular Solutions
- Solvation Gibbs Energy: The Equation of State Approach
- Limiting Activity Coefficients: New Procedures, Computations and Measurements
- Free Energy in Thermal and Chemical Protein Unfolding
- The Statistical Associating Fluid Theory
- Gibbs-Helmholtz Equation: Practical Applications in Thermochemistry
- Experimental Determination of Vapor Pressures
- Stability of Real Liquid Crystals
- Thermodynamics of the Folding and Interconversion of G-quadruplex DNA Structures

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Advance Book Information

Photochemistry
Volume 49

Stefano Crespi University of Groningen, The Netherlands
Stefano Protti University of Pavia, Italy

Synopsis
Reviewing photo-induced processes that have relevance to a wide number of academic and commercial disciplines, this volume reflects the current interests in chemistry, physics, biology and technology. The volume continues to provide essential reading for postgraduates, academics and industrialists working in the field of photochemistry, enabling them to keep on top of the literature.

Brief Contents
- Introduction of the year 2020
- The great schism in photochemistry
- The molecules of colour. The real blue indigo: photostability mechanisms, new functional derivatives, and hybrids
- Light induced reactions in cryogenic matrices (2019-2020)
- Photobiological systems studied by time-resolved infrared spectroscopy (2019-2020)
- Photophysics of transition metal complexes (2019-2020)
- Recent advances in photocatalytic water splitting and hydrogen generation (2019-2020)
- Solar photocatalysis for water decontamination and disinfection (2017-2020)
- C-C and C-Heteroatom bonds photocatalyzed and photoinitiated by carbonyls
- Excited-state symmetry breaking: from fundamental photophysics to asymmetrical photochemistry
- Recent applications of photoinduced decarboxylative radical reactions catalyzed by photoredox catalysts
- Selected applications of plasmonic nanoparticles in photosciences
- Enhancing Photosynthesis in organic biological hybrid complexes
- Porphyrins as photocatalysts in organic photoredox transformations
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Ion Mobility–Mass Spectrometry
Fundamentals and Applications

Alison E Ashcroft University of Leeds, UK
Frank Sobott University of Leeds, UK

Synopsis
Over the last decade, the use of ion mobility separation in combination
with mass spectrometry analysis has developed significantly. This
technique adds a unique extra dimension enabling the in-depth analysis
of a wide range of complex samples in the areas of the chemical and
biological sciences. Providing a comprehensive guide to the technique,
each chapter is written by an internationally recognised expert and with
numerous different commercial platforms to choose from, this book will
help the end users understand the practicalities of using different
instruments for different ion mobility purposes. The book is primarily
aimed at researchers appealing to practising chemists and biochemists
as well as those in the pharmaceutical and medical fields.

Brief Contents
- Ion Mobility–Mass Spectrometry: an Overview
- Calculation of Momentum Transfer Cross-sections
- Fundamentals of Uniform-field Drift Tube Ion Mobility and Collision
  Cross Section
- Travelling Wave Ion Mobility Separation: Basics and Calibration
- Trapped Ion Mobility Spectrometry – Basics and Calibration
- Field Asymmetric Ion Mobility Spectrometry (FAIMS) for Advanced
  Mass Spectrometry
- Computational Approaches for Processing Native Ion Mobility–Mass
  Spectrometry Data
- CCS for Modelling 3D Structures
- Ion Spectroscopy Coupled to Ion Mobility–Mass Spectrometry
- Ion Mobility–Mass Spectrometry of Pharmaceuticals
- Ion Mobility Spectrometry in Mass Spectrometry Imaging
- Ion Mobility–Mass Spectrometry in Metabolomics Studies
- The Role of Ion Mobility for Antibody Characterisation: A Biopharmaceutical
  Perspective