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Stuart G. Whittington
Editor

Numerical Methods for Polymeric Systems



Springer

Numerical Methods For Polymeric Systems

**Donald L. Wise, Gary E. Wnek, Debra J.
Trantolo, Thomas M. Cooper, Joseph D.
Gresser**

Numerical Methods For Polymeric Systems:

Numerical Methods for Polymeric Systems Stuart G. Whittington, 2012-12-06 Polymers occur in many different states and their physical properties are strongly correlated with their conformations. The theoretical investigation of the conformational properties of polymers is a difficult task and numerical methods play an important role in this field. This book contains contributions from a workshop on numerical methods for polymeric systems held at the IMA in May 1996 which brought together chemists, physicists, mathematicians, computer scientists and statisticians with a common interest in numerical methods. The two major approaches used in the field are molecular dynamics and Monte Carlo methods and the book includes reviews of both approaches as well as applications to particular polymeric systems. The molecular dynamics approach solves the Newtonian equations of motion of the polymer giving direct information about the polymer dynamics as well as about static properties. The Monte Carlo approaches discussed in this book all involve sampling along a Markov chain defined on the configuration space of the system. An important feature of the book is the treatment of Monte Carlo methods including umbrella sampling and multiple Markov chain methods which are useful for strongly interacting systems such as polymers at low temperatures and in compact phases. The book is of interest to workers in polymer statistical mechanics and also to a wider audience interested in numerical methods and their application in polymeric systems. Eco-friendly and Smart

Polymer Systems Hamid Mirzadeh, Ali Asghar Katbab, 2020-05-29 This proceedings book presents the main findings of the 13th International Seminar on Polymer Science and Technology ISPST 2018 which was held at Amirkabir University of Technology Tehran on November 10-22, 2018. This forum was the culmination of more than three decades of academic and industrial activities of Iranian scholars and professionals and the participation of many notable international scientists in covering various important polymer-related subjects of concern to Iran and the world at large including polymer synthesis, processing and properties as well as issues concerning polymer degradation, stability and environmental aspects. For the past half a century, the growing concern for advancing human health, quality of life and especially in the last few decades, avoiding and combating environmental pollution have shaped and driven scientific activities geared toward the creation of smart materials that are compatible with the human body and have prompted scientists and technologists to pursue research using natural and sustainable sources. This book highlights efforts to responsibly address the problems caused by and which can potentially be solved by polymers and plastics.

Statistical Physics of Polymers Toshihiro Kawakatsu, 2013-03-09 This book is an introductory textbook on the statistical mechanics of polymers and complex fluids aimed at senior undergraduate and graduate students and non-specialist researchers who are starting research in this field. Modern statistical mechanics on polymers and complex fluids is based on many fields such as chemical physics, statistical mechanics, quantum mechanics, stochastic processes, theory of phase transitions, hydrodynamics, rheology and so on. This book provides an overview of the basic concepts and methods used in current research on the physics of polymers and complex fluids. Using simple but

essential examples we describe how to derive the physical properties of polymers theoretically focusing on the structure and dynamics on mesoscopic scales Here the term mesoscopic scales means intermediate lengths and time scales between the microscopic atomic scale and the macroscopic scale Properties on mesoscopic scales are the central issue of the physics of polymers and complex fluids because these materials are well characterized by spatiotemporal structures on these scales where we can extract universal properties that are independent of the microscopic details of the system

Modeling and Simulation in Polymer Reaction Engineering Klaus-Dieter Hungenberg, Michael Wulkow, 2018-05-29 Introducing a unique modular approach to modeling polymerization reactions this useful book will enable practitioners chemists and engineers alike to set up and structure their own models for simulation software like Predici C MatLab or others The generic modules are exemplified for concrete situations for various reactor types and reaction mechanisms and allow readers to quickly find their own point of interest a highly useful information source for polymer engineers and researchers in industry and academia

Simulation Methods for Polymers Michael Kotelyanskii, Doros N. Theodorou, 2004-03-15 Synthetic Lubricants and High Performance Functional Fluids Second Edition offers state of the art information on all the major synthetic fluids describing established products as well as highly promising experimental fluids with commercial potential This second edition contains chapters on polyinternalolefins polymer esters refrigeration lubes polyphenyl ethers highly refined mineral oils automotive gear oils and industrial gear oils The book also assesses automotive industrial aerospace environmental and commercial trends in Europe Asia South America and the US

Photonic Polymer Systems Donald L. Wise, Gary E. Wnek, Debra J. Trantolo, Thomas M. Cooper, Joseph D. Gresser, 1998-07-10 Furnishes the necessary background information methods of characterization and applications of optic and photonic systems based on polymers Provides detailed tutorial chapters that offer in depth explanations of optic and photonic fundamentals and synthesis techniques

Chemorheology of Polymers Peter J. Halley, Graeme A. George, 2009-05-28 Understanding the dynamics of reactive polymer processes allows scientists to create new high value high performance polymers This book is an indispensable resource for researchers and practitioners working in this area It includes coverage of thermoplastics thermoset and reactive polymers together with practical industrial processes and modern chemorheological models and tools

Multiphase Polymer Systems Andreea Irina Barzic, Silvia Ioan, 2016-09-19 Phase morphology in multicomponent polymer based systems represents the main physical characteristic that allows for control of the material design and implicitly the development of new plastics Emphasizing properties of these promising new materials in both solution and solid phase this book describes the preparation processing properties and practical implications of advanced multiphase systems from macro to nanoscales It covers a wide range of systems including copolymers polymer blends polymer composites gels interpenetrating polymers and layered polymer metal structures describing aspects of polymer science engineering and technology The book analyzes experimental and theoretical aspects regarding the thermal and electrical transport phenomena and magnetic properties of

crucial importance in advanced technologies It reviews the most recent advances concerning morphological rheological interfacial physical fire resistant thermophysical and biomedical properties of multiphase polymer systems Concomitantly the book deals with basic investigation techniques that are sensitive in elucidating the features of each phase It also discusses the latest research trends that offer new solutions for advanced bio and nanotechnologies Introduces an overview of recent studies in the area of multiphase polymer systems their micro and nanostructural evolutions in advanced technologies and provides future outlooks new challenges and opportunities Discusses multicomponent structures that offer enhanced physical mechanical thermal electrical magnetic and optical properties adapted to current requirements of modern technologies Covers a wide range of materials such as composites blends alloys gels and interpenetrating polymer networks Presents new strategies for controlling the micro and nanomorphology and the mechanical properties of multiphase polymeric materials Describes different applications of multiphase polymeric materials in various fields including automotive aeronautics and space industry displays and medicine

Theory and Modeling of Polymer Nanocomposites Valeriy V. Ginzburg, Lisa M. Hall, 2020-12-16 This edited volume brings together the state of the art in polymer nanocomposite theory and modeling creating a roadmap for scientists and engineers seeking to design new advanced materials The book opens with a review of molecular and mesoscale models predicting equilibrium and non equilibrium nanoscale structure of hybrid materials as a function of composition and especially filler types Subsequent chapters cover the methods and analyses used for describing the dynamics of nanocomposites and their mechanical and physical properties Dedicated chapters present best practices for predicting materials properties of practical interest including thermal and electrical conductivity optical properties barrier properties and flammability Each chapter is written by leading academic and industrial scientists working in each respective sub field The overview of modeling methodology combined with detailed examples of property predictions for specific systems will make this book useful for academic and industrial practitioners alike

Mathematical Methods in Contemporary Chemistry Kuchanov, 1996-03-20

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