Chemical Equilibrium Utkstair

Suitable for advanced undergraduate and graduate students, this text presents the general properties of partial differential equations, including the elementary theory of complex variables. Solutions. 1965 edition.

Free energy constitutes the most important thermodynamic quantity to understand how chemical species recognize each other, associate or react. Examples of problems in which knowledge of the underlying free energy behaviour is required, include conformational equilibria and molecular association, partitioning between immiscible liquids, receptor-drug interaction, protein-protein and protein-DNA association, and protein stability. This volume sets out to present a coherent and comprehensive account of the concepts that underlie different approaches devised for the determination of free energies. The reader will gain the necessary insight into the theoretical and computational foundations of the subject and will be presented with relevant applications from molecular-level modelling and simulations of chemical and biological systems. Both formally accurate and approximate methods are covered using both classical and quantum mechanical descriptions. A central theme of the book is that the wide variety of free energy calculation techniques available today can be understood as different implementations of a few basic principles. The book is aimed at a broad readership of graduate students and researchers having a background in chemistry, physics, engineering and physical biology.

Both process planning and scheduling are very important functions of manufacturing, which affect together the cost to manufacture a product and the time to deliver it. This book contains various approaches proposed by researchers to integrate the process planning and scheduling functions of manufacturing under varying configurations of shops. It is useful for both beginners and advanced researchers to understand and formulate the Integration Process Planning and Scheduling (IPPS) problem effectively. Features Covers the basics of both process planning and scheduling Presents nonlinear approaches, closed-loop approaches, as well as distributed approaches Discuss the outfit of IPPS in Industry 4.0 paradigm Includes the benchmarking problems on IPPS Contains nature-algorithms and metaheuristics for performance measurements in IPPS Presents analysis of energy-efficient objective for sustainable manufacturing in IPPS

Understanding Molecular Simulation: From Algorithms to Applications explains the physics behind the "recipes" of molecular simulation for materials science. Computer simulators are continuously confronted with questions concerning the choice of a particular technique for a given application. A wide variety of tools exist, so the choice of technique requires a good understanding of the basic principles. More importantly, such understanding may greatly improve the efficiency of a simulation program. The implementation of simulation methods is illustrated in pseudocodes and their practical use in the case studies used in the text. Since the first edition only five years ago, the simulation world has changed significantly -- current techniques have matured and new ones have appeared. This new edition deals with these new developments; in particular, there are sections on: · Transition path sampling and diffusive barrier crossing to simulaterare events · Dissipative particle dynamic as a course-grained simulation technique · Novel schemes to compute the long-ranged forces · Hamiltonian and non-Hamiltonian dynamics in the context constant-temperature and constant-pressure molecular dynamics simulations · Multiple-time step algorithms as an alternative for constraints · Defects in solids · The pruned-enriched Rosenbluth sampling, recoil-growth, and concerted rotations for complex molecules · Parallel tempering for glassy Hamiltonians Examples are included that highlight current applications and the codes of case studies are available on the World Wide Web. Several new examples have been added since the first edition to illustrate recent applications. Questions are included in this new edition. No prior knowledge of computer simulation is assumed.

Free Energy CalculationsTheory and Applications in Chemistry and BiologySpringer Science & Business Media

Multicomponent Diffusion discusses the multicomponent diffusion of the three phases of matter. The book is comprised of nine chapters that cover studies of multicomponent diffusion and mass transfer with an emphasis on the chemical characteristics responsible for multicomponent diffusion. Chapter 1 provides an introductory discourse about multicomponent diffusion. Chapter 2 discusses binary diffusion, while Chapter 3 covers multicomponent flux equation. The measurement of ternary diffusion and the estimation of ternary diffusion coefficients are also explained in the book. A chapter then covers the interacting systems, and the subsequent chapter talks about membranes without mobile carriers. The text also discusses carrier-containing membranes and the multicomponent mass transfer. The book will be of great use to researchers and professionals whose work requires a good understanding of multicomponent diffusion.