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Cherry Magic! Thirty Years of Virginity Can Make You a Wizard?! 1 Yuu Toyota 2020-03-10 It's complicated: A thirty-year-old virgin gets more than he bargained for when his newfound magical power reveals he's the object of his male coworker's affections! Adachi, a thirty-year-old virgin, discovers he has the magical power to read the minds of people he touches. Unfortunately, the ability just makes him miserable since he doesn't know how to use it well! And to make matters worse, when he accidentally reads the mind of his very

competent, handsome colleague, Adachi discovers the guy has a raging crush on none other than Adachi himself! Things are about to get VERY awkward!

Spin Crossover in Transition Metal Compounds 2004

Current Issues In Nursing - E-Book Perle Slavik Cowen 2014-04-14 Current Issues in Nursing provides a forum for knowledgeable debate on the important issues that nurses face today. This resource provides the opportunity to analyze conflicting viewpoints and develop your own thoughts on demands being made for the nursing profession and the difficult issues affecting today's health care delivery. Continually praised for its in-depth discussion of critical issues, solid organization of material, and encouragement of independent thinking, you'll find this text a valuable resource in the modern world of nursing. Offers comprehensive and timely coverage of the issues affecting nursing education and practice. UNIQUE! Over 100 well-known contributors offer their expert insights and analysis. UNIQUE! Viewpoint chapters present controversial issues to showcase pressing issues facing nursing today. New content covering the following topics: The Challenges of Nursing on an International Level Health Care Systems and Practice Ethics, Legal, and Social Issues The Changing Practice Professional Challenges, Collaboration, & Conflict Violence Prevention and Care: Nursing's Role Definitions of Nursing Changing Education

Computational Chemistry David Young 2004-04-07 A practical, easily accessible guide for bench-top chemists, thisbook focuses on accurately applying computational chemistrytechniques to everyday chemistry problems. Provides nonmathematical explanations of advanced topics incomputational chemistry. Focuses

on when and how to apply different computationaltechniques. Addresses computational chemistry connections to biochemicalsystems and polymers. Provides a prioritized list of methods for attacking difficultcomputational chemistry problems, and compares advantages anddisadvantages of various approximation techniques. Describes how the choice of methods of software affectsrequirements for computer memory and processing time.

Soft Matter Systems for Biomedical Applications Leonid Bulavin 2021-09-27 This book addresses new challenges in soft matter and colloids. It presents timely reports on colloidal self-assembly, soft matters from liquid crystals, nanoparticles in liquid crystals, hydrocolloids, hybrid nanosystems, nanosuspensions, and dispersion of nanoparticles in different media, soft matter processing and modern experiments related with soft matters.

Dissertation Abstracts International 2005

σ- and π-Hole Interactions Antonio Frontera 2021-03-30 This book describes unconventional noncovalent interactions and analyzes their importance for crystal growth in organic and hybrid organic–inorganic systems. Several examples illustrate how the combination of theory and experiment allows rationalizing the strength and directionality of noncovalent interactions. This book elegantly describes the results of a survey of X-ray structures of main group element compounds (M = Sn, Pb As, Sb, Bi, and Te) exhibiting intermolecular M•••Se noncovalent interactions in one of its chapters. Moreover, it provides a consistent description of noncovalent interactions, covering most groups of the periodic table. The interactions are described and discussed using their trivial names. That is, a comprehensive and accurate description is

provided for alkali, alkaline earth, regium, spodium, triel, tetrel, pnictogen, chalcogen, halogen, and aerogen bonding interactions. No other book is available covering such an extensive number of interactions and examples where these interactions are relevant. relevant.

Recent Financial Crises The late Lawrence R. Klein 2007-01-01 Financial crises are recurring phenomena that can cause significant economic and societal loss. This book is therefore vitally important as it analyzes why and how financial crises occur, the extent of their impact, and what can be done to prevent their recurrence or reduce the damage they cause. Comprising original and never-before-published papers by distinguished economists, this book offers insights about lessons that were or should have been learned from recent outbreaks of such crises in East Asia and elsewhere. Recent Financial Crises also presents a set of econometric studies of issues such as labor market behavior, investment and productivity, and exchange rate adjustments. Although China did not have a crisis, its economic behavior was closely monitored in order to see if that had any effect on the crisis conditions. In this respect, the book contains an estimation of China s core inflation rate, as well as its true cost of living index, over a 20-year period spanning the Asian financial crisis. In general, collectively, the studies point to a need for ongoing structural reforms to minimize vulnerability to crises or soften their impact. The necessity for resorting to viable safety nets is also stressed. Policymakers and central bankers will find this book of great value, as will scholars and researchers at many levels of academe, involved in financial, business, and international economics.

Polymer Journal 2007

Machine Learning Meets Quantum Physics Kristof T. Schütt 2020-06-03 Designing molecules and materials with desired properties is an important prerequisite for advancing technology in our modern societies. This requires both the ability to calculate accurate microscopic properties, such as energies, forces and electrostatic multipoles of specific configurations, as well as efficient sampling of potential energy surfaces to obtain corresponding macroscopic properties. Tools that can provide this are accurate first-principles calculations rooted in quantum mechanics, and statistical mechanics, respectively. Unfortunately, they come at a high computational cost that prohibits calculations for large systems and long time-scales, thus presenting a severe bottleneck both for searching the vast chemical compound space and the stupendously many dynamical configurations that a molecule can assume. To overcome this challenge, recently there have been increased efforts to accelerate quantum simulations with machine learning (ML). This emerging interdisciplinary community encompasses chemists, material scientists, physicists, mathematicians and computer scientists, joining forces to contribute to the exciting hot topic of progressing machine learning and AI for molecules and materials. The book that has emerged from a series of workshops provides a snapshot of this rapidly developing field. It contains tutorial material explaining the relevant foundations needed in chemistry, physics as well as machine learning to give an easy starting point for interested readers. In addition, a number of research papers defining the current state-of-the-art are included. The book has five parts (Fundamentals, Incorporating Prior Knowledge, Deep Learning of Atomistic

Representations, Atomistic Simulations and Discovery and Design), each prefaced by editorial commentary that puts the respective parts into a broader scientific context.

Organic Reaction Mechanisms 2018 Mark G. Moloney 2021-08-17 Organic Reaction Mechanisms 2018, the 54th annual volume in this highly successful and unique series, surveys research on organic reaction mechanisms described in the available literature dated 2018. The following classes of organic reaction mechanisms are comprehensively reviewed: Reaction of Aldehydes and Ketones and their Derivatives Reactions of Carboxylic, Phosphoric, and Sulfonic Acids and their Derivatives Oxidation and Reduction Carbenes and Nitrenes Nucleophilic Aromatic Substitution Electrophilic Aromatic Substitution Carbocations Nucleophilic Aliphatic Substitution Carbanions and Electrophilic Aliphatic Substitution Elimination Reactions Polar Addition Reactions Cycloaddition Reactions Molecular Rearrangements Transition Metal Coupling Radical Reactions An experienced team of authors compile these reviews every year, so that the reader can rely on a continuing quality of selection and presentation.

Free Energy Computations Tony Leli□vre 2010 This monograph provides a general introduction to advanced computational methods for free energy calculations, from the systematic and rigorous point of view of applied mathematics. Free energy calculations in molecular dynamics have become an outstanding and increasingly broad computational field in physics, chemistry and molecular biology within the past few years, by making possible the analysis of complex molecular systems. This work proposes a new, general and rigorous presentation, intended both for practitioners

interested in a mathematical treatment, and for applied mathematicians interested in molecular dynamics.

Machine Learning in Chemistry Hugh M Cartwright 2020-07-15 Progress in the application of machine learning (ML) to the physical and life sciences has been rapid. A decade ago, the method was mainly of interest to those in computer science departments, but more recently ML tools have been developed that show significant potential across wide areas of science. There is a growing consensus that ML software, and related areas of artificial intelligence, may, in due course, become as fundamental to scientific research as computers themselves. Yet a perception remains that ML is obscure or esoteric, that only computer scientists can really understand it, and that few meaningful applications in scientific research exist. This book challenges that view. With contributions from leading research groups, it presents in-depth examples to illustrate how ML can be applied to real chemical problems. Through these examples, the reader can both gain a feel for what ML can and cannot (so far) achieve, and also identify characteristics that might make a problem in physical science amenable to a ML approach. This text is a valuable resource for scientists who are intrigued by the power of machine learning and want to learn more about how it can be applied in their own field.

Ab Initio Molecular Dynamics Dominik Marx 2009-04-30 Ab initio molecular dynamics revolutionized the field of realistic computer simulation of complex molecular systems and processes, including chemical reactions, by unifying molecular dynamics and electronic structure theory. This book provides the first coherent presentation of this rapidly growing field, covering a vast

range of methods and their applications, from basic theory to advanced methods. This fascinating text for graduate students and researchers contains systematic derivations of various ab initio molecular dynamics techniques to enable readers to understand and assess the merits and drawbacks of commonly used methods. It also discusses the special features of the widely used Car–Parrinello approach, correcting various misconceptions currently found in research literature. The book contains pseudo-code and program layout for typical plane wave electronic structure codes, allowing newcomers to the field to understand commonly used program packages and enabling developers to improve and add new features in their code.

My Imaginary Boyfriend Patrick Rangsimant 2020-06-25 "If you leave it without saying goodbye,it will come back to deprive the life out of you."At first, Phai though that Klong was only his imaginary friend who stepped up to be an imaginary boyfriend. But seems like Klong doesn't want to be only imagination, he wants to be more even he has to do something terrible... This is a paranormal thriller romantic novel about Phai who falls in with his imaginary friend whom he left behind without saying goodbye since he was young. After the reunion with Klong, even Phai feels really happy but there is a feeling that touches at the back of his neck. It's fear. Because it's like in the bedtime rhyme said about the imaginary friend "If you leave it without saying goodbye,it will come back to deprive the life out of you."

FUTURE FORWARD DUNCAN. CHATTHARAKUL MCCARGO (ANYARAT.) 2020

Probabilistic Machine Learning Kevin P. Murphy 2022-03-01 A detailed and up-to-date introduction to machine learning,

presented through the unifying lens of probabilistic modeling and Bayesian decision theory. This book offers a detailed and up-to-date introduction to machine learning (including deep learning) through the unifying lens of probabilistic modeling and Bayesian decision theory. The book covers mathematical background (including linear algebra and optimization), basic supervised learning (including linear and logistic regression and deep neural networks), as well as more advanced topics (including transfer learning and unsupervised learning). End-of-chapter exercises allow students to apply what they have learned, and an appendix covers notation. Probabilistic Machine Learning grew out of the author's 2012 book, Machine Learning: A Probabilistic Perspective. More than just a simple update, this is a completely new book that reflects the dramatic developments in the field since 2012, most notably deep learning. In addition, the new book is accompanied by online Python code, using libraries such as scikit-learn, JAX, PyTorch, and Tensorflow, which can be used to reproduce nearly all the figures; this code can be run inside a web browser using cloud-based notebooks, and provides a practical complement to the theoretical topics discussed in the book. This introductory text will be followed by a sequel that covers more advanced topics, taking the same probabilistic approach.

2gether vol. 2 (□□□□□□□□□□□□□□ 2 English Version) JittiRain / maggie mae 2020-06-19 " My name is Tine (a super chic guy), and I've gone out with all kinds of girls. A nerdy girl, a cute, innocent girl, or even a super grouchy girl. But then my joyous life has to come to a stop when the mighty god in the form of university admission sends me to a northern university where I get to meet… "Tine, Teepakorn, first-year Law student, I

like you!” Just the beginning of the first semester, someone already confesses to me. Am I surprised? Am I excited? Nah. Well, I’m such a cool guy, you know. But am I horrified? Hell yes! Because the one who just confessed to me is a dude!! My heart... The mission to shake off this huge gay dude out of my chic life starts with finding someone hella hot to be my fake boyfriend. And nobody fits the role as much as Sarawat, the nation’s husband of our university. But things aren’t as easy as I expected. This guy is a pain in the ass. He’s playing hard to get, not cooperating with me. Ha, I won’t give up that easily! Constant dropping wears away a stone. I’ll stick with him like a suckerfish. Just wait and see! But...as I’m pestering him, why the heck is my super chic heart starting to flutter when I’m with this straight-faced dude...? " keyword: □□□□□, □□□□□□□□, Thai novel, Thai ebook, hytexts, □□□□□□□, jamsaieverypub

Modern Quantum Chemistry Attila Szabo 2012-06-08 This graduate-level text explains the modern in-depth approaches to the calculation of electronic structure and the properties of molecules. Largely self-contained, it features more than 150 exercises. 1989 edition.

Routledge Handbook of Contemporary Thailand Pavin Chachavalpongpun 2019-11-08 The Routledge Handbook of Contemporary Thailand is a timely survey and assessment of the state of contemporary Thailand. While Thailand has changed much in the past decades, this handbook proposes that many of its problems have remained intact or even persistent, particularly problems related to domestic politics. It underlines emerging issues at this critical juncture in the kingdom and focuses on the history, politics, economy, society, culture, religion and international relations of the country. A

multidisciplinary approach, with chapters written by experts on Thailand, this handbook is divided into the following sections. History Political and economic landscape Social development International relations Designed for academics, students, libraries, policymakers and general readers in the field of Asian studies, political science, economics and sociology, this invaluable reference work provides an up-to-date account of Thailand and initiates new discussion for future research activities.

I Wanna Text You Up Teagan Hunter 2018-01-28 When I put up a ROOMMATE WANTED poster, he was the last person on earth I thought would respond.He was also the last person on earth I'd agree to let live with me...on purpose.But, here we are-roommates. I'm certain we can coexist without it being awkward, and I'm determined to make it work. There will be no sexual tension building with each accidental touch, no flutters when he wears that stupid backward baseball cap, and definitely no flirting when we text back and forth.Caleb Mills can't be the guy for me. He's my best friend's ex-boyfriend.And that would be wrong...right?

Biomolecular Simulations Massimiliano Bonomi 2020-08-14 This volume explores the recent advancements in biomolecular simulations of proteins, small molecules, and nucleic acids, with a primary focus on classical molecular dynamics (MD) simulations at atomistic, coarse-grained, and quantum/ab-initio levels. The chapters in this book are divided into four parts: Part One looks at recent techniques used in the development of physic-chemical models of proteins, small molecules, nucleic acids, and lipids; Part Two discusses enhanced sampling and free-energy calculations; Part Three talks about integrative computational and experimental approaches for

biomolecular simulations; and Part Four focuses on analyzing, visualizing, and comparing biomolecular simulations. Written in the highly successful Methods in Molecular Biology series format, chapters include introductions to their respective topics, lists of the necessary materials and reagents, step-by-step, readily reproducible laboratory protocols, and tips on troubleshooting and avoiding known pitfalls. Cutting-edge and comprehensive, Biomolecular Simulations: Methods and Protocols is a valuable resource for both novice and expert researchers who are interested in studying different areas of biomolecular simulations, and discovering new tools to progress their future projects.

Computational Science – ICCS 2018 Yong Shi 2018-06-11 The three-volume set LNCS 10860, 10861 + 10862 constitutes the proceedings of the 18th International Conference on Computational Science, ICCS 2018, held in Wuxi, China, in June 2018. The total of 155 full and 66 short papers presented in this book set was carefully reviewed and selected from 404 submissions. The papers were organized in topical sections named: Part I: ICCS Main Track Part II: Track of Advances in High-Performance Computational Earth Sciences: Applications and Frameworks; Track of Agent-Based Simulations, Adaptive Algorithms and Solvers; Track of Applications of Matrix Methods in Artificial Intelligence and Machine Learning; Track of Architecture, Languages, Compilation and Hardware Support for Emerging ManYcore Systems; Track of Biomedical and Bioinformatics Challenges for Computer Science; Track of Computational Finance and Business Intelligence; Track of Computational Optimization, Modelling and Simulation; Track of Data, Modeling, and Computation in IoT and Smart Systems;

Track of Data-Driven Computational Sciences; Track of Mathematical-Methods-and-Algorithms for Extreme Scale; Track of Multiscale Modelling and Simulation Part III: Track of Simulations of Flow and Transport: Modeling, Algorithms and Computation; Track of Solving Problems with Uncertainties; Track of Teaching Computational Science; Poster Papers

The Protein Folding Problem and Tertiary Structure Prediction Kenneth M.Jr. Merz 2012-12-06 A solution to the protein folding problem has eluded researchers for more than 30 years. The stakes are high. Such a solution will make 40,000 more tertiary structures available for immediate study by translating the DNA sequence information in the sequence databases into three-dimensional protein structures. This translation will be indispensable for the analy sis of results from the Human Genome Project, de novo protein design, and many other areas of biotechnological research. Finally, an in-depth study of the rules of protein folding should provide vital clues to the protein fold ing process. The search for these rules is therefore an important objective for theoretical molecular biology. Both experimental and theoretical ap proaches have been used in the search for a solution, with many promising results but no general solution. In recent years, there has been an exponen tial increase in the power of computers. This has triggered an incredible outburst of theoretical approaches to solving the protein folding problem ranging from molecular dynamics-based studies of proteins in solution to the actual prediction of protein structures from first principles. This volume attempts to present a concise overview of these advances. Adrian Roitberg and Ron Elber describe the locally enhanced sam pling/simulated annealing

conformational search algorithm (Chapter 1), which is potentially useful for the rapid conformational search of larger molecular systems.

Essentials of Computational Chemistry Christopher J. Cramer 2013-04-29 Essentials of Computational Chemistry provides a balanced introduction to this dynamic subject. Suitable for both experimentalists and theorists, a wide range of samples and applications are included drawn from all key areas. The book carefully leads the reader thorough the necessary equations providing information explanations and reasoning where necessary and firmly placing each equation in context.

Biomarkers in Psychiatry Judith Pratt 2019-01-05 This volume addresses one of the Holy Grails in Psychiatry, namely the evidence for and potential to adopt 'Biomarkers' for prevention, diagnosis, and treatment responses in mental health conditions. It meshes together state of the art research from international renowned pre-clinical and clinical scientists to illustrate how the fields of anxiety disorders, depression, psychotic disorders, and autism spectrum disorder have advanced in recent years.

The Effects of the Thai Economic Crisis and of Thai Labor Market Policies on Labor Market Outcomes Jere R. Behrman 2000

Mathematical Reviews 2002

Computational Modelling and Simulation of Materials II Pietro Vincenzini 2003

Catalysis for Clean Energy and Environmental Sustainability K. K. Pant 2021-05-13 This book is part of a two-volume work that offers a unique blend of information on realistic evaluations of catalyst-based synthesis processes using green chemistry principles and the environmental sustainability applications of

such processes for biomass conversion, refining, and petrochemical production. The volumes provide a comprehensive resource of state-of-the-art technologies and green chemistry methodologies from researchers, academics, and chemical and manufacturing industrial scientists. The work will be of interest to professors, researchers, and practitioners in clean energy catalysis, green chemistry, chemical engineering and manufacturing, and environmental sustainability. This volume focuses on the potentials, recent advances, and future prospects of catalysis for biomass conversion and value-added chemicals production via green catalytic routes. Readers are presented with a mechanistic framework assessing the development of product selective catalytic processes for biomass and biomass-derived feedstock conversion. The book offers a unique combination of contributions from experts working on both lab-scale and industrial catalytic processes and provides insight into the use of various catalytic materials (e.g., mineral acids, heteropolyacid, metal catalysts, zeolites, metal oxides) for clean energy production and environmental sustainability.

Handbook of Polymer Crystallization Ewa Piorkowska 2013-07 "The only comprehensive reference on polymer crystallization, Handbook of Polymer Crystallization provides readers with a broad, in-depth guide on the subject, covering the numerous problems encountered during crystallization as well as solutions to resolve those problems to achieve the desired result."--Provided by publisher.

Fundamentals of Deep Learning Nikhil Buduma 2017-05-25 With the reinvigoration of neural networks in the 2000s, deep learning has become an extremely active

area of research, one that's paving the way for modern machine learning. In this practical book, author Nikhil Buduma provides examples and clear explanations to guide you through major concepts of this complicated field. Companies such as Google, Microsoft, and Facebook are actively growing in-house deep-learning teams. For the rest of us, however, deep learning is still a pretty complex and difficult subject to grasp. If you're familiar with Python, and have a background in calculus, along with a basic understanding of machine learning, this book will get you started. Examine the foundations of machine learning and neural networks Learn how to train feed-forward neural networks Use TensorFlow to implement your first neural network Manage problems that arise as you begin to make networks deeper Build neural networks that analyze complex images Perform effective dimensionality reduction using autoencoders Dive deep into sequence analysis to examine language Learn the fundamentals of reinforcement learning

Transition Metals in Coordination Environments Ewa Broclawik 2019-03-16 This book focuses on the electronic properties of transition metals in coordination environments. These properties are responsible for the unique and intricate activity of transition metal sites in bio- and inorganic catalysis, but also pose challenges for both theoretical and experimental studies. Written by an international group of recognized experts, the book reviews recent advances in computational modeling and discusses their interplay using experiments. It covers a broad range of topics, including advanced computational methods for transition metal systems; spectroscopic, electrochemical and catalytic properties of transition metals in

coordination environments; metalloenzymes and biomimetic compounds; and spin-related phenomena. As such, the book offers an invaluable resource for all researchers and postgraduate students interested in both fundamental and application-oriented research in the field of transition metal systems.

Khaki Capital Paul Chambers 2017

Problem-Solving Therapy Thomas D'Zurilla, PhD 2006-09-18 MAXIMIZE POSITIVE PATIENT OUTCOMES Enhance Function--Avert Relapses--Present New Problems In this new updated edition, authors Thomas J. D'Zurilla and Arthur M. Nezu, present some of the most useful advances in problem-solving therapy (PST) today. An excellent resource for maximizing positive patient outcomes, this all-inclusive guide helps enhance your problem solving skills and apply successful clinical techniques to help your clients improve their lives. Known for its presentation of solid research results and effective PST training tools, this best-selling guide has been fully updated to include: NEW research data on social problem solving and adjustment NEW studies on the efficacy of PST NEW social problem solving models NEW updated and more user-friendly therapist's training manual Written for a wide audience, from therapists and counselors to psychologists and social workers, this highly readable and practical reference is a must-have guide to helping your patients identify and resolve current life problems. The book set is designed to be read alongside its informal "manual" accompaniment, Solving Life's Problems: A 5-Step Guide to Enhanced Well-Being by D'Zurilla, Nezu, and Christine Maguth Nezu. Purchase of the two books as a set will get you these life-changing texts at an $7.00 savings over the two books bought individually.

Mathematical Analysis With Applications Sandra Pinelas 2020-05-26 This proceedings volume covers research in key areas of applied mathematical analysis, and gathers works presented at the international conference “Concord-90,” in honor of the 90th birthday of Professor Constantin Corduneanu (1928-2018). The event – which Professor Corduneanu was able to attend – was held at Ural Federal University in Ekaterinburg, Russia, on July 26-28, 2018. Professor Corduneanu’s research in mathematical analysis spanned nearly seven decades and explored a range of important issues in the field, including studies of global existence, stability problems, and oscillation theory, with special emphasis on various classes of nonlinear equations. He published over two hundred articles and several books, including “Almost Periodic Oscillations and Waves” (Springer, 2009). In this volume the reader will find selected, peer-reviewed articles from seven fields of research – Differential Equations, Optimal Control and Stabilization; Stochastic Methods; Topology and Functions Approximation; Mathematical Biology and Bioinformatics; Mathematical Modeling in Mining; Mathematical Modeling in Economics; and Computer Science and Image Processing – which honor and reflect Professor Corduneanu’s legacy in the fields of oscillation, stability and control theory.

TDRI Quarterly Review 2001

Social Media in Travel, Tourism and Hospitality Evangelos Christou 2016-04-01 Social media is fundamentally changing the way travellers and tourists search, find, read and trust, as well as collaboratively produce information about tourism suppliers and tourism destinations. Presenting cutting-edge theory, research and case studies investigating Web 2.0 applications and tools that transform the role and behaviour of the

new generation of travellers, this book also examines the ways in which tourism organisations reengineer and implement their business models and operations, such as new service development, marketing, networking and knowledge management. Written by an international group of researchers widely known for their expertise in the field of the Internet and tourism, chapters include applications and case studies in various travel, tourism and leisure sectors.

Classical and Quantum Dynamics in Condensed Phase Simulations Bruce J Berne 1998-06-17 The school held at Villa Marigola, Lerici, Italy, in July 1997 was very much an educational experiment aimed not just at teaching a new generation of students the latest developments in computer simulation methods and theory, but also at bringing together researchers from the condensed matter computer simulation community, the biophysical chemistry community and the quantum dynamics community to confront the shared problem: the development of methods to treat the dynamics of quantum condensed phase systems. This volume collects the lectures delivered there. Due to the focus of the school, the contributions divide along natural lines into two broad groups: (1) the most sophisticated forms of the art of computer simulation, including biased phase space sampling schemes, methods which address the multiplicity of time scales in condensed phase problems, and static equilibrium methods for treating quantum systems; (2) the contributions on quantum dynamics, including methods for mixing quantum and classical dynamics in condensed phase simulations and methods capable of treating all degrees of freedom quantum-mechanically. Contents:Barrier Crossing: Classical Theory of Rare but

Important Events (D Chandler)Monte Carlo Simulations (D Frenkel)Molecular Dynamics Methods for the Enhanced Sampling of Phase Space (B J Berne)Constrained and Nonequilibrium Molecular Dynamics (G Ciccotti & M Ferrario)From Erying to Kramers: Computation of Diffusive Barrier Crossing Rates (M J Ruiz-Montero)Monte Carlo Methods for Sampling of Rare Event States (W Janke)Proton Transfer in Ice (D Marx)Nudged Elastic Band Method for Finding Minimum Energy Paths of Transitions (H Jónsson et al.)RAW Quantum Transition State Theory (G Mills et al.)Dynamics of Peptide Folding (R Elber et al.)Theoretical Studies of Activated Processes in Biological Ion Channels (B Roux & S Crouzy)The Semiclassical Initial Value Representation for Including Quantum Effects in Molecular Dynamics Simulations (W H Miller)Tunneling in the Condensed Phase: Barrier Crossing and Dynamical Control (N Makri)Feynman Path Centroid Methods for Condensed Phase Quantum Dynamics (G A Voth)Quantum Molecular Dynamics Using Wigner Representation (V S Filinov et al.)Nonadiabatic Molecular Dynamics Methods for Diffusion (D Laria et al.)and other papers Readership: Computational and statistical physicists. Keywords:Quantum;Molecular Dynamics;DynamicsReviews: “… this volume is a useful introduction to currently popular, and widely-used techniques in chemical and statistical physics. The authors are well-respected researchers in the field and the level is appropriate to graduate students and researchers.” Journal of Statistical Physics

Microfiltration and Ultrafiltration Zeman 2017-11-22 Integrates knowledge on microfiltration and ultrification, membrane chemistry, and characterization methods with the engineering and economic aspects

of device performance, device and module design, processes, and applications. The text provides a discussion of membrane fundamentals and an analytical framework for designing and developing new filtrations systems for a broad range of technologically important functions. It offers information on membrane liquid precursors, fractal and stochastic pore space analysis, novel and advanced module designs, and original process design calculations.