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Dennis R. Salahub,Dongqing Wei

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Multiscale Dynamics Simulations Dennis R. Salahub, Dongqing Wei, 2021-09-24 Over the past decade, great strides have been taken in developing methodologies that can treat more and more complex nano- and nano-bio systems embedded in complex environments. Multiscale Dynamics Simulations covers methods including DFT/MM-MD, DFTB and semi-empirical QM/MM-MD, DFT/MMPOL as well as Machine-learning approaches to all of the above. Focusing on key methodological breakthroughs in the field, this book provides newcomers with a comprehensive menu of multiscale modelling options so that they can better chart their course in the nano/bio world.

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Crises, Contagion, and the Closed Mr. Angel J. Ubide, Mr. Eduardo Levy Yeyati, 1998-09-01 This paper analyzes the behavior of closed-end country fund discounts, including evidence from the Mexican and East Asian crises. We find that the ratio of fund prices to their fundamental value increases dramatically during a crisis, an anomaly that we denote the "closed-end country fund puzzle." Our results show that the puzzle relates directly to the fact that international investors are less (more) sensitive to changes in local (global) market conditions than domestic investors. This asymmetry implies that foreign participation in local markets can both help dampen a crisis in the originating country, and amplify the contagion to noncrisis countries.

The Textual Tradition of Plato's Republic Gerard Boter, 2018-08-14

Introductory Medical Statistics, 3rd edition Richard F. Mould, 1998-01-01 Introductory Medical Statistics, now in its third edition, is an introductory textbook on basic statistical techniques. It is written for physicians, surgeons, radiation oncologists, medical physicists, radiographers, hospital administrators, medical statisticians in training, biochemists, and other professionals allied to medicine. It is suitable

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Metallic Systems Thomas C. Allison, Orkid Coskuner, Carlos A. Gonzalez, 2011-05-09 Metallic systems are ubiquitous in daily life. They play key roles, for example, in the chemistry of many biomolecules, ionic solutions, nanoparticles, and catalytic processes. They may be in solid, liquid, or gaseous form. The interactions of other molecules with metal surfaces are of considerable importance. Each of these topics is addressed in M

Concepts and Methods in Modern Theoretical Chemistry, Two Volume Set Swapan Kumar Ghosh, Pratim Kumar Chattaraj, 2020-06-16 Concepts and Methods in Modern Theoretical Chemistry, Two-Volume Set focuses on the structure and dynamics of systems and phenomena. A new addition to the series Atoms, Molecules, and Clusters, the two books offer chapters written by experts in their fields. They enable readers to learn how concepts from ab initio quantum chemistry, density functio

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Computer Aided Systems Theory - EUROCAST '97 Franz Pichler, Franz Pichler (Ing., Dr. phil.), Roberto Moreno-Diaz, 1997-11-05 This book constitutes a refereed post-workshop selection of papers presented at the 6th International Workshop on Computer-Aided Systems Theory, EUROCAST'97, held in Las Palmas de Gran Canaria, Spain, in February 1997. The 50 revised full papers presented were carefully selected for inclusion in the volume. The book is divided into sections on design environments and tools, theory and methods, engineering systems, intelligent systems, signal processing, and specific methods and applications.

Data Transportation and Protection John E. Hershey, Rao K. Yarlagadda, 2012-12-06 A new breed of engineer is developing in our contemporary

society. These engineers are concerned with communications and computers, economics and regulation. These new engineers apply themselves to data-to its pack aging, transmission, and protection. They are data engineers. Formal curricula do not yet exist for their dedicated development. Rather they learn most of their tools on the job and their roots are in computer engineering, communications engineering, and applied mathematics. There is a need to draw relevant material together and present it so that those who wish to become data engineers can do so, for the betterment of themselves, their employer, their country, and, ultimately, the world-for we share the belief that the most effective tool for world peace and stability is neither politics nor armaments, but rather the open and timely exchange of information. This book has been written with that goal in mind. Today numerous signs encourage us to expect broader information exchange in the years to come. The movement toward a true Integrated Services Digital Network (ISDN) is perhaps the clearest of these. Also, the development of formal protocol layers reflects both a great deal of brilliance and compromise and also the desire for a common language among data engineers.

Molecular Electronic Structures of Transition Metal Complexes II David Michael P. Mingos, Peter Day, Jens Peder Dahl, 2012-01-11 This book reviews current and future trends in modern chemical research, focusing on chemical structure and bonding. Covers development of electronic structure theories for transition metal complexes, orbital models and electronic structure theory and more.

Optical Modeling and Simulation of Thin-Film Photovoltaic Devices Janez Krc, Marko Topic, 2016-04-19 In wafer-based and thin-film photovoltaic (PV) devices, the management of light is a crucial aspect of optimization since trapping sunlight in active parts of PV devices is essential for efficient energy conversions. Optical modeling and simulation enable efficient analysis and optimization of the optical situation in optoelectronic and PV devices.

Electrocardiology '96: From The Cell To The Body Surface: Proceedings Of The Xxiii International Congress On Electrocardiology J Liebman, 1997-07-01 This conference had as its focus the phrase 'From the Cell to the Body Surface'. It comprised five minisymposia, which concentrated on some of the major issues of the day for basic scientists and clinicians. In addition to the invited papers, the proceedings contain volume presentations and posters selected from among abstracts sent in by some of the most important investigators in electrocardiology worldwide.

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