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Larissa V. Chernysheva

Computation of Atomic and Molecular Processes

Introducing the ATOM-M Software Suite



 Springer

Computation Of Atomic Structure And Processes

Mark Steyvers



Computation Of Atomic Structure And Processes:

Computation of Atomic and Molecular Processes Miron Ya. Amusia, Larissa V. Chernysheva, 2021-12-02 This book presents numerical methods for solving a wide range of problems associated with the structure of atoms and simplest molecules and their interaction with electromagnetic radiation electrons and other particles It introduces the ATOM M software package presenting a unified software suite written in Fortran for carrying out precise atomic and molecular numeric calculations The book shows how to apply these numerical methods to obtain many different characteristics of atoms molecules and the various processes within which they interact In an entirely self sufficient approach it teaches the reader how to use the codes provided to build atomic and molecular systems from the ground up and obtain the resulting one electron wave functions The computational programs presented and made available in this book allow calculations in the one electron Hartree Fock approximation and take into account many electron correlations within the framework of the random phase approximation with exchange or many body perturbation theory Ideal for scholars interested in numerical computation of atomic and molecular processes the material presented in this book is useful to both experts and novices theorists and experimentalists

Computational Atomic Structure Charlotte Froese-Fischer, T Brage, 1997-01-01 Computational Atomic Structure An MCHF Approach deals with the field of computational atomic structure specifically with the multiconfiguration Hartree Fock MCHF approach and the manner in which this approach is used in modern physics Beginning with an introduction to computational algorithms and procedures for atomic physics the book describes the theory underlying nonrelativistic atomic structure calculations making use of Breit Pauli corrections for relativistic effects and details how the MCHF atomic structure software package can be used to this end The book concludes with a treatment of atomic properties such as energy levels electron affinities transition probabilities specific mass shift fine structure hyperfine structure and autoionization This modern reliable exposition of atomic structure theory proves invaluable to anyone looking to make use of the authors MCHF atomic structure software package which is available publicly via the Internet

Methods in Computational Chemistry Stephen Wilson, 2013-12-14 Providing specialist reviews and analyses of contemporary theories algorithms and techniques this series aims to facilitate the effective exploitation of available computing power The current volume focuses on the theoretical determination of atomic and molecular properties as related to wave functions electron densities and total energies

Supercomputing, Collision Processes, and Applications Kenneth L. Bell, Keith A. Berrington, Derrick S.F. Crothers, Alan Hibbert, Kenneth T. Taylor, 2006-04-18 Professor Philip G Burke CBE FRS formally retired on 30 September 1998 To recognise this occasion some of his colleagues friends and former students decided to hold a conference in his honour and to present this volume as a dedication to his enormous contribution to the theoretical atomic physics community The conference and this volume of the invited talks reflect very closely those areas with which he has mostly been associated and his influence internationally on the development of atomic physics coupled with

a parallel growth in supercomputing Phil's wide range of interests include electron atom molecule collisions scattering of photons and electrons by molecules adsorbed on surfaces collisions involving oriented and chiral molecules and the development of non perturbative methods for studying multiphoton processes His development of the theory associated with such processes has enabled important advances to be made in our understanding of the associated physics the interpretation of experimental data has been invaluable in application to fusion processes and the study of astrophysical plasmas observed by both ground and space based telescopes We therefore offer this volume as our token of affection and respect to Philip G Burke with the hope that it may also fill a gap in the literature in these important fields

Comprehensive Biophysics

,2012-04-12 Biophysics is a rapidly evolving interdisciplinary science that applies theories and methods of the physical sciences to questions of biology Biophysics encompasses many disciplines including physics chemistry mathematics biology biochemistry medicine pharmacology physiology and neuroscience and it is essential that scientists working in these varied fields are able to understand each other's research Comprehensive Biophysics Nine Volume Set will help bridge that communication gap Written by a team of researchers at the forefront of their respective fields under the guidance of Chief Editor Edward Egelman Comprehensive Biophysics Nine Volume Set provides definitive introductions to a broad array of topics uniting different areas of biophysics research from the physical techniques for studying macromolecular structure to protein folding muscle and molecular motors cell biophysics bioenergetics and more The result is this comprehensive scientific resource a valuable tool both for helping researchers come to grips quickly with material from related biophysics fields outside their areas of expertise and for reinforcing their existing knowledge Biophysical research today encompasses many areas of biology These studies do not necessarily share a unique identifying factor This work unites the different areas of research and allows users regardless of their background to navigate through the most essential concepts with ease saving them time and vastly improving their understanding The field of biophysics counts several journals that are directly and indirectly concerned with the field There is no reference work that encompasses the entire field and unites the different areas of research through deep foundational reviews Comprehensive Biophysics fills this vacuum being a definitive work on biophysics It will help users apply context to the diverse journal literature offering and aid them in identifying areas for further research Chief Editor Edward Egelman E I C Biophysical Journal has assembled an impressive world class team of Volume Editors and Contributing Authors Each chapter has been painstakingly reviewed and checked for consistent high quality The result is an authoritative overview which ties the literature together and provides the user with a reliable background information and citation resource

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International Conference on Computational Physics (ICCP ...), 1993 **The Progress of Atomic Theory** Albert Cushing
 Crehore, 1926 **Atomic Structure Theory** Walter R. Johnson, 2007-02-05 This book provides a hands on experience with
 atomic structure calculations Material covered includes angular momentum methods the central field Schrödinger and Dirac
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 Hartree Fock equations *Computational Methods in Classical and Quantum Physics* Michael Buchanan Hooper, Institute of
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Materials and Processes for Advanced CMOS: Volume 745 Mark I. Gardner, Materials Research Society, 2003-03-25
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