

Equation-of-motion coupled-cluster calculations
of photodetachment cross sections
for atomic negative ions across the periodic table

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Atomic Coupledcluster Calculations

Christian Drosten



Atomic Coupledcluster Calculations:

Atomic Coupled-cluster Calculations Anders Ynnerman, 1992

Recent Progress in Coupled Cluster Methods

Petr Cársky, Josef Paldus, Jirí Pittner, 2010-07-03 I feel very honored that I have been asked to write a Foreword to this book. The subject of the book Coupled cluster theory has been around for about half a century. The basic theory and explicit equations for closed shell ground states were formulated before 1970. At the beginning of the seventies the first ab initio calculations were carried out. At that time speed and memory of computers were very limited compared to today's standards. Moreover the size of one electron bases employed was small so that it was only possible to achieve an orientation in methodical aspects rather than to generate new significant results. Extensive use of the coupled cluster method started at the beginning of the eighties. With the help of more powerful computers the results of coupled cluster approaches started to yield more and more interesting results of relevance to the interpretation of experimental data. New ideas in methodology kept appearing and computer codes became more and more efficient. This exciting situation continues to this very day. Remarkably enough even the required equations can now be generated by a computer with the help of symbolic languages. The size of this monograph and the rich variety of articles it contains attests to the usefulness and viability of the coupled cluster formalism for the handling of many electron correlation effects. This represents a vivid testimony of a tremendous work that has been accomplished in coupled cluster methodology and its exploitation.

Atoms, Molecules And Clusters In Electric Fields:

Theoretical Approaches To The Calculation Of Electric Polarizability George Maroulis, 2006-07-31 With the central importance of electric polarizability and hyperpolarizability for a wide spectrum of activities this book charts the trends in the accurate theoretical determination of these properties in specialized fields. The contributions include reviews and original papers that extend from methodology to applications in specific areas of primary importance such as cluster science and organic synthesis of molecules with specific properties.

Computational Methods in Lanthanide and Actinide Chemistry

Michael Dolg, 2015-02-17 The f elements and their compounds often possess an unusually complex electronic structure governed by the high number of electronic states arising from open f shells as well as large relativistic and electron correlation effects. A correct theoretical description of these elements poses the highest challenges to theory. Computational Methods in Lanthanide and Actinide Chemistry summarizes state of the art electronic structure methods applicable for quantum chemical calculations of lanthanide and actinide systems and presents a broad overview of their most recent applications to atoms, molecules and solids. The book contains sixteen chapters written by leading experts in method development as well as in theoretical investigations of f element systems. Topics covered include Relativistic configuration interaction calculations for lanthanide and actinide anions. Study of actinides by relativistic coupled cluster methods. Relativistic all electron approaches to the study of f element chemistry. Relativistic pseudopotentials and their applications. Gaussian basis sets for lanthanide and actinide elements. Applied computational actinide chemistry. This book will serve as a

comprehensive reference work for quantum chemists and computational chemists both those already working in and those planning to enter the field of quantum chemistry for f elements Experimentalists will also find important information concerning the capabilities of modern quantum chemical methods to assist in the interpretation or even to predict the outcome of their experiments Advanced Topics in Theoretical Chemical Physics J. Maruani,Roland Lefebvre,Erkki J. Brändas,2013-11-27 Advanced Topics in Theoretical Chemical Physics is a collection of 20 selected papers from the scientific presentations of the Fourth Congress of the International Society for Theoretical Chemical Physics ISTCP held at Marly le Roi France in July 2002 Advanced Topics in Theoretical Chemical Physics encompasses a broad spectrum in which scientists place special emphasis on theoretical methods in chemistry and physics The chapters in the book are divided into five sections I Advances Chemical Thermodynamics II Electronic Structure of Molecular Systems III Molecular Interaction and Dynamics IV Condensed Matter V Playing with Numbers This book is an invaluable resource for all academics and researchers interested in theoretical quantum or statistical chemical physics or physical chemistry It presents a selection of some of the most advanced methods results and insights in this exciting area **Relativistic Quantum Chemistry** Markus Reiher,Alexander Wolf,2015-01-12 Einstein proposed his theory of special relativity in 1905 For a long time it was believed that this theory has no significant impact on chemistry This view changed in the 1970s when it was realized that nonrelativistic Schrodinger quantum mechanics yields results on molecular properties that depart significantly from experimental results Especially when heavy elements are involved these quantitative deviations can be so large that qualitative chemical reasoning and understanding is affected For this to grasp the appropriate many electron theory has rapidly evolved Nowadays relativistic approaches are routinely implemented and applied in standard quantum chemical software packages As it is essential for chemists and physicists to understand relativistic effects in molecules the first edition of Relativistic Quantum Chemistry The fundamental Theory of Molecular Science had set out to provide a concise comprehensive and complete presentation of this theory This second edition expands on some of the latest developments in this fascinating field The text retains its clear and consistent style allowing for a readily accessible overview of the complex topic It is also self contained building on the fundamental equations and providing the mathematical background necessary While some parts of the text have been restructured for the sake of clarity a significant amount of new content has also been added This includes for example an in depth discussion of the Brown Ravenhall disease of spin in current density functional theory and of exact two component methods and its local variants A strength of the first edition of this textbook was its list of almost 1000 references to the original research literature which has made it a valuable reference also for experts in the field In the second edition more than 100 additional key references have been added most of them considering the recent developments in the field Thus the book is a must have for everyone entering the field as well as for experienced researchers searching for a consistent review Many-Body Methods for Atoms and Molecules Rajat Kumar Chaudhuri,Sudip Kumar

Chattopadhyay, 2017-02-17 Brings Readers from the Threshold to the Frontier of Modern Research Many Body Methods for Atoms and Molecules addresses two major classes of theories of electron correlation the many body perturbation theory and coupled cluster methods It discusses the issues related to the formal development and consequent numerical implementation of the methods from the standpoint of a practicing theoretician The book will enable readers to understand the future development of state of the art multi reference coupled cluster methods as well as their perturbative counterparts The book begins with an introduction to the issues relevant to the development of correlated methods in general It next gives a formally rigorous treatment of aspects that pave the foundation toward the theoretical development of methods capable of tackling problems of electronic correlation The authors go on to cover perturbation theory first in a fundamental way and then in the multi reference context They also describe the idea of state specific theories Fock space based multi reference coupled cluster methods and basic issues of the single reference coupled cluster method The book concludes with state of the art methods of modern electronic structure The 4th International Conference on Exotic Nuclei and Atomic Masses Carl J. Gross, Witold Nazarewicz, Krzysztof P. Rykaczewski, 2007-12-10 The International Conference on Exotic Nuclei and Atomic Masses ENAM has gained the status of the premier meeting for the physics of nuclei far from stability The selected and refereed papers presenting the main results constitute valuable proceedings that offer everyone working in this field an authoritative and comprehensive source of reference **New Electron Correlation Methods and their Applications, and Use of Atomic Orbitals with Exponential Asymptotes**, 2021-09-28 Advances in Quantum Chemistry presents surveys of current topics in this rapidly developing field one that has emerged at the cross section of the historically established areas of mathematics physics chemistry and biology It features detailed reviews written by leading international researchers In this volume the readers are presented with an exciting combination of themes Presents surveys of current topics in this rapidly developing field that has emerged at the cross section of the historically established areas of mathematics physics chemistry and biology Features detailed reviews written by leading international researchers Scientific and Technical Aerospace Reports, 1993

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