Lecture Notes in Chemistry 116

Cleanthes A. Nicolaides

**State- and Property-Specific Quantum Chemistry and Physics I**

Framework for the Many-Electron Calculation of Properties of Discrete and of Resonance States

This book, the first volume of a two-part monograph, is centered on key background fundamentals and results, and on the description of the State- and Property-Specific Approach (SPSA) to the construction and implementation of efficacious methods for the quantitative solution of various types of time-independent or time-dependent problems in Quantum Chemistry and in Atomic, Molecular, Optical, and Chemical Physics. By going beyond the standard many-electron problem for ground states, the discussion mainly addresses the key aspects of the SPSA methodology for the calculation of wavefunctions of excited discrete states and of resonance (autoionizing) states that are tailored to each property or phenomenon of interest. In particular, the SPSA uses state-specific function spaces and practicable computational methods that allow insightful and economic descriptions of excited-state electronic structures and the systematic calculation of the interplay between electronic structures (including electron correlations) on the one hand and spectra and dynamics on the other. The Hamiltonians (nonrelativistic or relativistic) are either field-free or include weak or strong electromagnetic fields that may be static, or periodic, or pulsed. The arguments and commentary in both volumes of the monograph are supported by a plethora of numerical examples and by comparisons with experiment.

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**State- and Property-Specific Quantum Chemistry and Physics II**

Theory and Calculation of Spectra and Dynamics. Field-Free and Field-Induced Nonstationary States

This book, the second volume of a two-part monograph, consists mainly of State- and Property-Specific Approach (SPSA) formulations for the efficient calculation of properties and of phenomena in N-electron atoms and molecules. Its bulk deals with nonperturbative solutions of the many-electron, time-independent, or time-dependent Schrödinger equations using Hermitian or non-Hermitian (complex energy) constructions that account consistently for the contribution of both the discrete and the multichannel continuous spectra. It covers a wide range of applications, including the prediction of spectra and properties of excited discrete and resonance (autoionizing, autodissociating) states, the construction of diabatic molecular states and their use in real systems for solving problems of reaction and of molecular bonding, multiphoton ionization and dissociation (including tunneling), field-induced partial and total energy shifts and decay rates, properties of negative ions in ground or excited open-shell states, ultrafast electron dynamics and electron rearrangements on femtosecond and attosecond timescales, and other topics.

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