Advances in Quantum Chemistry

Volume 64



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Jan Awrejcewicz

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Advances in Quantum Systems in Chemistry, Physics, and Biology Liliana Mammino, Davide Ceresoli, Jean Maruani, Erkki Brändas, 2020-02-05 This edited multi author book gathers selected peer reviewed contributions based on papers presented at the 23rd International Workshop on Quantum Systems in Chemistry Physics and Biology QSCP XXIII held in Mopani Camp The Kruger National Park South Africa in September 2018 The content is primarily intended for scholars researchers and graduate students working at universities and scientific institutes who are interested in the structure properties dynamics and spectroscopy of atoms molecules biological systems and condensed matter **Quantum Molecular Dynamics** David A. Micha, 2025-10-31 Presents theoretical computational and practical aspects of collision induced phenomena with emphasis on the treatment of physical and chemical kinetics using quantum molecular dynamics Quantum Molecular Dynamics provides a state of the art overview of molecular collisions for energy transfer and reactivity phenomena in gases Grounded in the quantal theory of scattering and its semiclassical limits this comprehensive volume covers key concepts and theory computational approaches and various applications for specific physical systems Detailed chapters describe elastic inelastic and reactive collisions that lead to energy transfer electronic transitions chemical reactions and more Starting from the electronic structure and atomic conformation of molecules the text proceeds from introductory material to advanced modern treatments relevant to applications to new materials the environment biological phenomena and energy and fuels production Provides a thorough introduction to collision dynamics with realistic intermolecular forces Covers thermal rates and cross sections of molecular collisions phenomena Examines electronic excitation and relaxation phenomena mediated by molecular collisions Discusses many atom scattering theory as an introduction to more advanced descriptions Presents the computational aspects required to calculate and compare cross sections with experimental data Includes worked examples and applications to different physical systems Quantum Molecular

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