



Electron Dynamics in Molecular Interactions :Principles and Applications

Frank Hagelberg

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This volume provides a comprehensive introduction to the theory of electronic motion in molecular processes — an increasingly relevant and rapidly expanding segment of molecular quantum dynamics. Emphasis is placed on describing and interpreting transitions between electronic states in molecules as they occur typically in cases of reactive scattering between molecules, photoexcitation or nonadiabatic coupling between electronic and nuclear degrees of freedom.

Electron Dynamics in Molecular Interactions aims at a synoptic presentation of some very recent theoretical efforts to solve the electronic problem in quantum molecular dynamics, contrasting them with more traditional schemes. The presented models are derived from their roots in basic quantum theory, their interrelations are discussed, and their characteristic applications to concrete chemical systems are outlined. This volume also includes an assessment of the present status of electron dynamics and a report on novel developments to meet the current challenges in the field.

Further, this monograph responds to a need for a systematic comparative treatise on nonadiabatic theories of quantum molecular dynamics, which are of considerably higher complexity than the more traditional adiabatic approaches and are steadily gaining in importance. This volume addresses a broad readership ranging from physics or chemistry graduate students to specialists in the field of theoretical quantum dynamics.

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