



Quantum Theory & Applications of Chemical Reaction Dynamics

John Zh Zhang

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This text provides a detailed presentation of modern quantum theories for treating the reaction dynamics of small molecular systems. Its main focus is on the development of successful quantum dynamics theories and computational methods for studying the molecular reactive scattering process, with specific applications given in detail for a number of benchmark chemical reaction systems in the gas phase and the gas surface. It deals with both the development and the application of the modern reactive or rearrangement scattering theory and is written in a fashion in which the development of the reactive scattering theory is closely coupled with its computational aspects for practical applications for realistic molecular reactions. The volume includes such topics as: methods for calculating rovibrational states of molecules; fundamental quantum theory for scattering (nonreactive and reactive); modern time-independent computational methods for reactive scattering; general time-dependent wave packet methods for reactive scattering; dynamic theory of chemical reactions; dynamics of molecular fragmentation; semiclassical description of quantum mechanics; and also some useful appendices.

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