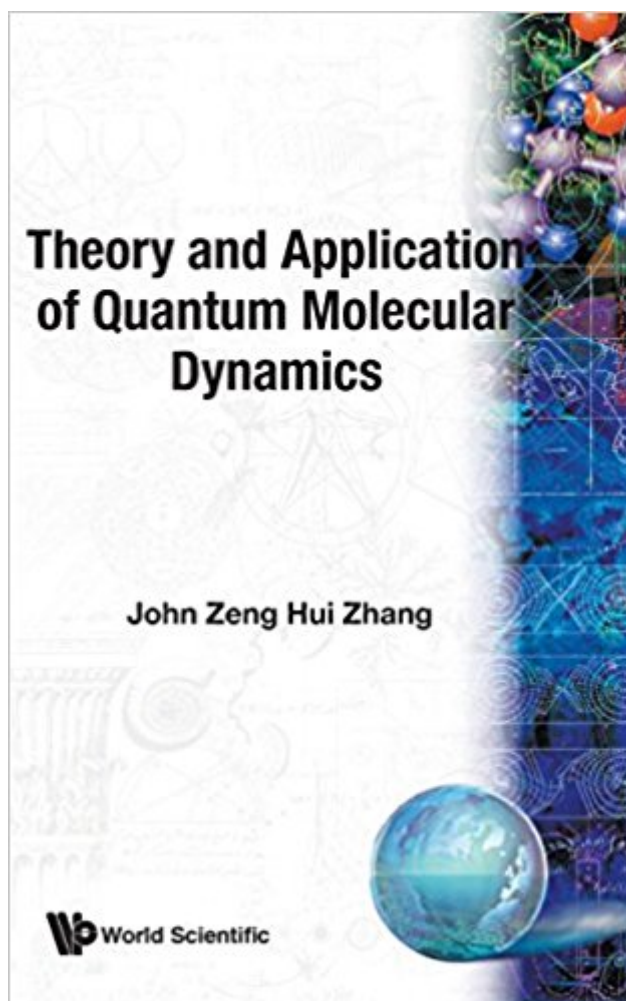


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THEORY AND APPLICATION OF QUANTUM MOLECULAR DYNAMICS



Synopsis

This book provides a detailed presentation of modern quantum theories for treating the reaction dynamics of small molecular systems. Its main focus is on the recent 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. In contrast to traditional books on collision in physics focusing on abstract theory for nonreactive scattering, this book 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, dynamics theory of chemical reactions, dynamics of molecular fragmentation, semiclassical description of quantum mechanics, and also some useful appendices. The book is intended for the reader to not only understand the molecular reaction dynamics from the fundamental scattering theory, but also utilize the provided computational methodologies in their practical applications. It should benefit graduate students and researchers in the field of chemical physics. Â

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