



Theories of Molecular Reaction Dynamics: The Microscopic Foundation of Chemical Kinetics (Oxford Graduate Texts)

Niels E. Henriksen, Flemming Y. Hansen

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This book deals with a central topic at the interface of chemistry and physics- the understanding of how the transformation of matter takes place at the atomic level. Building on the laws of physics, the book focuses on the theoretical framework for predicting the outcome of chemical reactions. The style is highly systematic with attention to basic concepts and clarity of presentation.

Molecular reaction dynamics is about the detailed atomic-level description of chemical reactions. Based on quantum mechanics and statistical mechanics, or, as an approximation, classical mechanics, the dynamics of uni- and bi-molecular elementary reactions are described. The book features a detailed presentation of transition-state theory which plays an important role in practice, and a comprehensive discussion of basic theories of reaction dynamics in condensed phases. Examples and end of chapter problems are included in order to illustrate the theory and its connection to chemical problems.

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