1. Record Nr. UNINA9910780043503321

Titolo	Theoretical methods in condensed phase chemistry [[electronic resource] /] / edited by Steven D. Schwartz
Pubbl/distr/stampa	Dordrecht ; ; Boston, : Kluwer Academic Publishers, c2000
ISBN	1-280-20546-6 9786610205462 0-306-46949-9
Edizione	[1st ed. 2002.]
Descrizione fisica	1 online resource (318 p.)
Collana	Progress in theoretical chemistry and physics ; ; v. 5
Altri autori (Persone)	SchwartzSteven David
Disciplina	541/.0421
Soggetti	Chemistry, Physical and theoretical Condensed matter
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Description based upon print version of record.
Nota di bibliografia	Includes bibliographical references and index.
Nota di contenuto	Classical and Quantum Rate Theory for Condensed Phases -- Feynman Path Centroid Dynamics -- Proton Transfer in Condensed Phases: Beyond the Quantum Kramers Paradigm -- Nonstationary Stochastic Dynamics and Applications to Chemical Physics -- Orbital-Free Kinetic-Energy Density Functional Theory -- Semiclassical Surface Hopping Methods for Nonadiabatic Transitions in Condensed Phases -- Mechanistic Studies of Solvation Dynamics in Liquids -- Theoretical Chemistry for Heterogeneous Reactions of Atmospheric Importance. The HC1+CIONO2 Reaction on Ice -- Simulation of Chemical Reactions in Solution Using an AB Initio Molecular Orbital-Valence Bond Model -- Methods for Finding Saddle Points and Minimum Energy Paths.
Sommario/riassunto	This book is meant to provide a window on the rapidly growing body of theoretical studies of condensed phase chemistry. A brief perusal of physical chemistry journals in the early to mid 1980’s will find a large number of theor- ical papers devoted to 3-body gas phase chemical reaction dynamics. The recent history of theoretical chemistry has seen an explosion of progress in the devel- ment of methods to study similar properties of systems with Avogadro’s number of particles. While the physical properties of condensed phase systems have long been principle targets of statistical mechanics, microscopic dynamic

theories that start from detailed interaction potentials and build to first principles predictions of properties are now maturing at an extraordinary rate. The techniques in use range from classical studies of new Generalized Langevin Equations, semicl- sical studies for non-adiabatic chemical reactions in condensed phase, mixed quantum classical studies of biological systems, to fully quantum studies of m-els of condensed phase environments. These techniques have become sufficiently sophisticated, that theoretical prediction of behavior in actual condensed phase environments is now possible. and in some cases, theory is driving development in experiment. The authors and chapters in this book have been chosen to represent a wide variety in the current approaches to the theoretical chemistry of condensed phase systems. I have attempted a number of groupings of the chapters, but the - versity of the work always seems to frustrate entirely consistent grouping.