



S.D. Schwartz (Ed.)

Theoretical Methods in Condensed Phase Chemistry

Series: Progress in Theoretical Chemistry and Physics

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 theoretical papers devoted to 3-body gas phase chemical reaction dynamics. The recent history of theoretical chemistry has seen an explosion of progress in the development 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, semiclassical studies for non-adiabatic chemical reactions in condensed phase, mixed quantum classical studies of biological systems, to fully quantum studies of models 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 diversity of the work always seems to frustrate entirely consistent grouping.

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