

Preface

Chemical reaction dynamic calculations provide the important information that can hardly be detected directly during the chemical elementary reaction dynamic processes by experimental means. Hence, dynamic simulations in atom and molecular level are conducive to reveal the basic rules and microscopic mechanism of the chemical reactions. Moreover, charge transfer process is the essential part of many chemical reactions in the fields of scientific research and industrial production. To explore the intrinsic mechanism of the intra- or inter-molecular charge transfer process will possess great realistic and scientific significance.

This special issue contains six papers in the field of atomic and molecular science. These selected papers deal with the theoretical descriptions of the stereodynamics for several important elementary reactions. Prof. Wei theoretically investigated the influence of the reactant vibrational excitation to the stereodynamics of the reaction $C + NO \rightarrow CN + O$, which is relevant to astrochemistry and NO reburning. Pro. Yue and coworkers dedicated effort to state-to-state dynamics analysis of the reaction $Li + HF(v=0, j=0) \rightarrow LiF(v', j') + H$ via the quasiclassical trajectory method. They mainly concern about the angular and rovibrational state distributions of the products. The paper by Pro. Meng *et al.* focuses on the dependence of the product polarization on collision energies of the reaction $Au + H_2(v=0, j=0) \rightarrow AuH + H$. Pro. Wang and coworkers studied the reverse reaction $H + NeH^+(v=0, j=0) \rightarrow H + NeH^+$ containing rare gas atoms. The influence of the collision energies to the reaction stereodynamics is discussed in detail. Using the method of coherence switching with decay of mixing (CSDM), Pro. Chen and coworkers theoretically studied the non-adiabatic dynamics processes for the reaction $Na(3s) + H_2 \rightarrow NaH(X^1\Sigma^+) + H$. By comparing the dynamics processes between adiabatic and non-adiabatic reactions, the significant influences of the integral cross sections to the reaction are revealed. The last paper by Pro. Song and Pro. Ma. analyzes the photoinduced charge transfer process of the organic donor-acceptor dyad in organic solar cells based on time-dependent density functional theory. Comparing the charge difference density, electronic coupling, reorganization energy and Gibbs free energy of the system, the significance of the external electric field to the charge transfer process is demonstrated.

We express deeply the gratitude to the authors who sent us their research articles. We also appreciate the enormous efforts from the journal and the reviewers. Their full support making this special issue present. We hope that this issue will attract more attentions to the microscopic mechanism of the chemical reactions, and then inspire more researchers to continue and improve their studies in this field.