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Preface

Symposium on the Frontier of Molecular Reaction Dynamics

This special issue of Journal of Atomic and Molecular Sciences describes the history and selected papers from the Conference on Symposium on the Frontier of Molecular Reaction Dynamics (CSFMRD), a series of national conferences suggested by Prof. Keli Han, who comes from the State Key Laboratory of Molecular Reaction Dynamics of the Chinese Academy of Sciences (SKLMRD-CAS). As a pioneer of chemical dynamics study in China, Prof. Han's group have done many important works in the fields of physics, chemistry, biology and material science, which has been widely recognized by international peers. They can provide scientists a powerful collection of integrated computing related resources and services-supercomputers, storage systems, software, visualization, and spectra technical support provided by experts including scientists and engineers. Thus, the conference was proposed and organized for promoting and improving the communications between the Chinese theoretical chemistry, computational chemistry, photochemistry, material chemistry community and their international counterparts.

1 THE FIRST AND PREVIOUSCONFERENCES

The first conference was held on September 23-25, 2011, in Dalian Institute of Chemical Physics, Chinese Academy of Sciences (DICP-CAS), and Prof. Keli Han was invited to be the chairperson. This conference attracted more than 30 attendees from 17 institutes and universities in China. 26 reports were given, and topics of lectures covered quantum control, drug molecular design, electronic structure, dynamics, supercomputing, renewable energy research, etc. As planned, the second and third conferences were held on June 15-17, 2012 and August 18-21, 2013, in Shanxi Normal University and Ludong University, respectively. These two conferences exchanged the research status, the latest achievements of molecular reaction dynamics in recent years. Also we explored the future development direction of this field. The topics mainly focused on the establishment of accurate potential energy surface by *ab initio* method, the new algorithm and method for calculating the molecular reaction dynamic process, the new progress in the experimental study of molecular reaction dynamics and the recent development and research results of molecular reaction dynamics and its related interdisciplinary.

2 CSFMRD4

The conference became more international after CSFMRD invited Professor Chaoyuan Zhu, a computational chemist from Institute of molecular Science, Department of Applied Chemistry, National Chiao Tung University, Hsinchu, Taiwan, to give a lecture in the fourth conference. It was held by Department of Physics, Liaoning University, on August 2-5, 2014, in the northern city of Shenyang. Department of Physics of Liaoning University has Liaoning Key Laboratory of Semiconductor Light Emitting and Photocatalytic Materials (LKLSLEPM) and Shenyang Key Laboratory of Optoelectronic Materials and Technology (SKLOMT). Based on these two Key Laboratories, they have done some meaningful works in the field of excited-state charge transfer dynamics, interaction of H-bond, photoelectric functional materials, etc. More than 60 experts attended this meeting, and 31 reports were given. The topic of the given talk covered the excited-state dynamics, nano materials, photophysics and photochemistry, development of supercomputing method, renewable energy research, etc.

At the meeting, Professor Fengcai Ma's group reviewed their recent advances in electronic excited-state proton transfer dynamics and the significant role of electronic excited-state hydrogen bonding on photoinduced electron transfer (PET), fluorescence quenching (FQ), intramolecular charge transfer (ICT). The combination of various spectroscopic experiments with theoretical calculations has led to tremendous progress in excited-state intramolecular proton transfer (ESIPT) reaction research. They investigated the novel excited-state proton transfer mechanisms of some simple dye molecules based on the time-dependent density functional theory (TDDFT). In addition, the proton transfer process provides a possible explanation for the fluorescence quenching observed.

Professor Tianshu Chu's presentation focused on the theoretical study of atom and electron motion in intense elliptically/circularly polarized laser filed. She introduced the proposed 3D-sine-DVR method: theory and test, and improvement in computational efficiency of 3D-sine-DVR method by introducing Wigner rotation technique. She also presented 3D quantum approach for studying the atom-laser interaction, and their calculated electron spectrum has good agreement with experimental result. By comparison, the computational efficiency of the 3D-sine-DVR method has been improved by introducing the Wigner rotation technique, and the agreement with previous experimental and theoretical studies has been proved to be good.

Professor Ruifeng Lu from Nanjing University of Science & Technology introduced their theoretical investigation on harmonic generation driven by intense midinfrared lasers. A valleylike structure is observed at very low-order harmonics because of a low-energy photoelectron suppression effect. Further, at the beginning of a broad supercontinuum, a convex structure appears that is distributed from the tail in a very narrow energy band in time-frequency maps. Surprisingly, their quantum dynamics calculations demonstrated the beneficial wavelength scaling of the harmonic yield to be $\lambda^{4.6}$ for He and $\lambda^{5.1}$ for Ne over selected energy windows. The bandwidth of the harmonic plateau with only a single quantum trajectory contribution can be further extended by adding a

controlling laser field, and the harmonic efficiency is found to be significantly enhanced after macroscopic propagation. In addition, ultrashort isolated attosecond pulses can be obtained by properly superposing the harmonics in the plateaus of both the He and Ne systems.

Professor Qiang Wei from Chongqing University of Technology presented a talk on quasiclassical trajectory study of stereodynamics for exchange reactions H′(D′) +H(D)S. He introduced their calculated results on the product polarizations for the exchange reaction H′+HS and its isotopic variants on an accurate 1A′ potential energy surface at collision energies of 10 kcal/mol. In addition, they discussed the product rotational angular momentum distributions $P(\theta_r)$ and $P(\phi_r)$ in the center-of-mass (CM) frame, and three generalized polarization-dependent differential cross sections (PDDCSs) of this kind of reaction. Their results demonstrated that the isotopic effect displays sensitive effect on the product vector correlations.

Professor Chunyuan Hou from Anhui Polytechnic University presented a talk on how the quantum mechanical approach were used to investigate the antioxidative mechanism for scavenging $^{\bullet}$OOH and $^{\bullet}$OH radicals using mangiferin in solution phase. Their calculated results indicated that the 7-OH site of mangiferin is important in the antioxidant activity, and the oxidation of mangiferin by $^{\bullet}$OOH and $^{\bullet}$OH radical is an exothermic process. The predicted maximum electron mobility value of mangiferin appears at the orientation angle near $49^{\circ}/311^{\circ}$ of conducting channel on the reference planes a-b. Their theoretical investigation of natural semiconductors is helpful for designing higher performance electronic materials used in biochemical and industrial field to replace expensive and rare organic materials.

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