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# Preface

*Institute of Atomic and Molecular Physics, Jilin University*

This special issue preface of Journal of Atomic and Molecular Sciences describes the history and main research areas of Institute of Atomic and Molecular Physics (IAMP), Jilin University. Moreover, this preface presents the works published in this special issue of Journal of Atomic and Molecular Sciences.

## 1 THE HISTORY AND RESEARCH AREAS OF IAMP

The Institute of Atomic and Molecular Physics (IAMP) in Jilin University is the first institution for graduated education and research in atomic and molecular physics in China, which is established in 1979 authorized by the State Ministry of Education, China. Nowadays IAMP has becomes a center of innovative science and technology for ultrafast intense laser interaction with matters, structural and dynamic theory of atoms and molecules, quantum manipulation of atomic and molecular processes, and material physics under extremer high pressure.

## 2 THE WORKS IN THIS SPECIAL ISSUE

Professor Ying Shi investigated excited state intramolecular proton transfer (ESIPT) process of 2-hydroxypyrene-1-carbaldehyde (HC). The geometric structures of HC system and its tautomer in both the ground state $S_0$ and the lowest singlet excited state $S_1$ were globally optimized at B3LYP/TZVP theoretical level. Simultaneously, the vertical single state excitation energy, corresponding to the oscillator strengths in different electronic states, and the frontier molecular orbitals (MOs) were presented. Further verification of the occurrence of proton transfer reaction was also implemented via IR spectra and potential energy curve. The results show that the intramolecular hydrogen bond is significantly strengthened in $S_1$ state, which provide a driving force in facilitates the ESIPT reaction. Furthermore, the electron density distributions of MOs were demonstrated to be a positive factor for the ESIPT. Finally, a reasonable deactivation mechanism for the excited state of HC system was successfully achieved.

Professor Bing Yan *et al.* investigated the vibrational and rotational spectroscopic constants of $X^1\Sigma^+$ for NaH and also reported rotation-vibration spectra of the ground state for the isotopes of NaH, NaD and NaT molecules. High-level *ab initio* calculations

 

utilizing explicitly correlated multi-reference configuration interaction method (MRCI-F12), considering Davidson modification(Q), core-valence correlation correction(CV) and scalar relativistic correction(SR), were performed to compute the Born-Oppenheimer potential energy curve (PEC) of the ground state $X^1\Sigma^+$ of NaH. The equilibrium internuclear distances $R_e$ and dissociation energies $D_e$ were calculated to be 1.8865Å and 15823.29cm$^{-1}$ for the ground state $X^1\Sigma^+$ of NaH, which are in good agreement with the experimental results of 1.8859Å and 15815$\pm$5cm$^{-1}$.

Professor Xue-Shen Liu *et al.* theoretically demonstrated the generation of high-order harmonic and attosecond pulse in the near-infrared (IR) laser field by adding a terahertz controlling pulse. The Lewenstein model is applied to investigate the high-order harmonic generation of He atom in the two-color field with the ground depletion taken into account. The time-frequency analysis, the three-step model and the ionization rate calculated by ADK model is applied to illustrate the physical mechanism of HHG. The scheme makes it possible for HHG quantum paths manipulation and only the short path is selected, making the spectrum in second plateau broader and smoother. By superposing a proper range of harmonic spectrum, we obtain an isolated attosecond pulse with the duration of 71 as.

Associate professor Jing Guo *et al.* investigated the high-order-harmonic generation (HHG) from three dimensional (3D) Hydrogen atom in ultraviolet (UV)-assisted chirped fields by solving the time-dependent Schrödinger equation (TDSE) accurately with time-dependent generalized pseudospectral (TDGPS) method. The results show that the HHG spectra is greatly broadened and enhanced when a 128 nm UV pulse is added on a chirped fundamental field, which is quite similar as the HHG from H atom initially prepared in the first excited state in the chirped field only. Besides, the HHG of H atom in the combination of a chirped fundamental field and a 256 nm UV pulse case is also investigated. The HHG process is illustrated by the semi-classical three-step model and the time-frequency analysis. The ionization probability and electron wavepacket as functions of time are also calculated to further illustrate this phenomenon. Furthermore, the influence of time delay between the chirped fundamental field and the 128 nm UV pulse on HHG process is also discussed. Finally, by superposing the harmonics in the range of 200th-260th order, an isolated attosecond pulse with a duration of about 64 as can be generated.

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