

Preface

College of Physics and Electronic Engineering, Henan Normal University

This special issue preface of Journal of Atomic and Molecular Sciences describes the history and main research areas of Atomic and Molecular subject from College of Physics and Electronic Engineering, Henan Normal University. This preface presents the works published in this special issue of Journal of Atomic and Molecular Sciences.

1 THE HISTORY OF COLLEGE OF PHYSICS AND ELECTRONIC ENGINEERING

The history of the College of Physics and Electronic Engineering, Henan normal University dates back to 1923, which is one of time-honored and larger scale department. Now it set tree departments (The physics department, electronic information engineering department, pedagogy department) and two research laboratory (Theoretical Physics Laboratory and Applied Physics Laboratory), which have the theoretical physics doctor station and physics first-level discipline master pilot. As the first-level key discipline, physics subject recruits master in 1978 and obtain the master authorized location in 1986. And from 1988, it is awarded the first level key subject of Henan province six years. From 2003, College of Physics unites the Chinese Academy of Sciences to graduate doctor students and obtain the theoretical physics doctor authorized location in 2006. The physic subject obtains the first batch physics national specialty development in 2007 and the physics first-level doctor authorized location in 2010. Now the physics subject includes the physics first-level doctor location (theoretical physic, particle physics and nuclear physics, atomic and molecular physics, condensed matter physics, optics, radio physic, plasma physics and acoustics second master location), the physics postdoctoral research station, the physics first-level master location, the physics provincial key subject and the key laboratory of photovoltaic materials in Henan province.

The atomic and molecular physics is the Advantage subject in physics first-level key discipline. From 1992, the subject start training master students, and turn into the sixth master authorized subject in 1996. In 2001, the subject has jointed recruit doctor students and become the Henan provincial key subject in 2004. The College of Physics and Electronic Engineering is one of the member units in the Atomic and molecular Professional Committee which is the most authoritative domestic organization for this subject.

In recent years, more than 20 well-known experts and scholars both from home and abroad including Professor Dajun Ding from the Institute of Atomic and Molecular Physics

at Jilin University, research fellow Jianmin Yuan from the National University of Defense Technology, Chinese Academy of Sciences, research fellow Keli Han from the Dalian Institute of Chemical Physics, Chinese Academy of Sciences, and research fellow Jianguo Wang from the Institute of Wuhan Institute of physics and Mathematics, research fellow Xiaoxin Zhou from the Northwest Normal University, and so on. Subject members and students will attend the relevant conferences, such as XXVIII International Conference on Photonic, Electronic and Atomic Collisions, National Academic Conference of Atomic and Molecular Physics, International Symposium of Theoretical and Computational Physical Chemistry, Symposium on Frontier of Molecular Reaction Dynamics and so on.

There are two main research fields in Atomic and Molecular subject. The first one is the study of atomic molecular collision: 1. Electron and atom molecule collision; 2. Electron and atom collision in laser field; 3. Atom and molecule collision. The second one is the molecular structure, spectra and excited state dynamics research: 1. Construction of potential energy function; 2. Excited state dynamics analysis; 3. Study on carrier mobility of organic semiconductor.

2 THE WORKS IN THIS SPECIAL ISSUE

Professor Yufang Liu focuses on the properties of $N_1-H_1 \cdots O_1$ hydrogen bond of N-methylaniline-DMSO complex (complex I) and N-methylaniline-acetone complex (complex II) in the excited state. The infrared spectra are in good agreement with the experiment data. The analysis of the bond length and AIM (atoms in molecules) demonstrated that the $N_1-H_1 \cdots O_1$ hydrogen bond is weakening from DMSO to acetone in the ground state. That is to say, the intermolecular hydrogen bond $N_1-H_1 \cdots O_1$ between N-methylaniline and solvent molecular is stronger with the polarity of solvent stronger. Upon photoexcitation, the analysis of AIM implies that the intermolecular complex II is enhanced. Interestingly, the hydrogen bond $N_1-H_1 \cdots O_1$ of complex I is weakened. The analysis of molecular orbital also support the results that the intermolecular hydrogen bond $N_1-H_1 \cdots O_1$ of complex I is weakened whereas it of complex II is enhanced.

Doctor Hongsheng Zhai and coworkers have studied the BSe^+ ion at the level of aug-cc-PVQZ basis set. The calculated electronic states, including four triple and two quintuple N-S states, are correlated to the dissociation limit of $B^+(^1S_g)+Se(^3P_g)$ and $B(^2P_u)+Se+(^4S_u)$. The states of $^3\Pi(II)$ and $^3\Sigma^-(II)$ from the dissociation limit of $Se^+(^4S_u)+B(^2P_u)$ both have double well and spectroscopic properties are studied. Various curve crossing are revealed, which could lead to the predissociation of the $X^3\Pi$ and $^5\Pi$ states and the possible predissociation pathway are analyzed. Spin-orbit coupling interaction is taken into account via the state interaction approach with the full Breit-Pauli Hamiltonian operator, which causes the entire six Λ -S states to split into 21 Ω states. This is the first time spin-orbit coupling calculation of BSe^+ . The potential energy curves of the Λ -S and Ω electronic states are depicted with the aid of the avoided crossing rule between electronic states of the same symmetry. Then the spectroscopic constants of bound Λ -S and Ω states

were obtained, which have never been observed in experiment.

Doctor Jian Song has investigated several fluorescent protein fluorophores with regular substitution in gas phase using TDDFT with long range corrected functional. Absorption and emission of both neutral and anionic chromophore states were calculated. The spectral shift amplitudes of calculation are in good agreement with experiment. The further intramolecular charge transfer process analysis show that conjugated area, charge transfer number/distance and transfer efficiency can affect spectral shift. Specially, the "N" atom with lone pair electrons of conjugated ring has an important influence on charge transfer process, and the conjugated length between hydroxyl and bridge bond only impact the anionic spectral shift. Our results about fluorescent chromophore spectral red shift mechanism do provide positive clues on new experimental far-red fluorescent protein designing.

Doctor Kedong Wang has studied low-energy electron collision with methylamine using *R*-matrix approach within the static-exchange (SE) and static-exchange-polarization (SEP) approximations. The elastic integral, momentum transfer and differential cross sections are reported. The calculated elastic integral cross sections are in agreement with the available experimental and theoretical data. A σ^* shape resonances of $^2A'$ symmetry located at 8.9 eV are detected within SEP model. For this dipole molecule Born-closure procedure was used to account for the higher partial waves ($l > 4$) to obtain the convergence of the cross section.

Doctor Dapeng Yang *et al.* investigated the excited state intramolecular proton transfer (ESIPT) process in aid of the time-dependent density functional theory (TDDFT) method. The geometric structures, frontier molecular orbitals, electrostatic potential (ESP) maps as well as the absorption and fluorescence spectra of the two forms of the title compound have been investigated. The calculated absorption spectra of the Keto form are more in agreement with the experimental results. Moreover, the potential energy curves of the intramolecular proton transfer (IPT) within the title compound have been scanned in both ground states S_0 and the first excited state S_1 . We found that the intramolecular proton transfer from Enol form to Keto form in excited state is almost barrierless with an energy barrier 2.1 kJ/mol whereas intramolecular proton transfer between the two forms of the title compound in ground state is forbidden with energy barrier as high as 10.5 kJ/mol.

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Notes

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