J. At. Mol. Sci

Vol. **6**, No. 2, pp. i-iii
June 2015

Preface

Atomic and Molecular Physics Laboratory, Ludong University

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

1 THE HISTORY OF AMPL

AMPL was established in 1997. It has been strongly supported by Ludong University in terms of financial funding and talent introduction and become one of the most important laboratories in Shandong province. The laboratory obtained the special funding of the Shandong Province Government in 2002. The master degree authorization of atomic and molecular Physics was gained in 2003, and the postgraduate students were enrolled in 2004. In July 2005, the laboratory was awarded as the Key laboratory in Universities of Shandong Province. In October 2006, the laboratory was further awarded as the Shandong Province key laboratory of atomic and molecular physics in the 11th Five-Year Plan. Keli Han, Professor in the Dalian Institute of Chemical Physics of Chinese Academy of Science, is hired as the director of the Academy Committee of AMPL. Professor Chuanlu Yang acts as the laboratory director.

In recent years, more than 50 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 Mingsheng Zhan from the Wuhan Institute of Physics and Mathematics, 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 Applied Physics and Computational Mathematics are invited to the laboratory and exchange academic thoughts. The 1st International Symposium of Theoretical and Computational Physical Chemistry (2005), the 2nd National Conference of Calculated Atomic and Molecular Physics (2008), the 3rd Symposium on Frontier of Molecular Reaction Dynamics (2013), the 6th Conference of the 7th Committee on Atomics and Molecular Physics of the Chinese Physical Society (2014), the 18th National Academic Conference of Atomics and Molecular Physics (2015) were hosted by AMPL.

2 THE RESEARCH AREAS OF AMPL

There are four main research fields in AMPL: cluster and nanostructure, interaction between laser and atoms or molecules, device and technology of photoelectric material, and molecular reaction dynamics. Being the academic frontier field, these research fields have achieved unique research characteristics. These fields strongly connect with each other. Based on them, a research system which is capable of understanding the relation between the structure and performance of the matter at atomic and molecular level, and designing and producing nano device and nano material with new functionalities, is constructed. The laboratory has over 600 square meters working space, and 25 million RMB in total value of the equipment.

The laboratory has Sugon 4000A super computer, HP-LH6000 server. In experimental research, there are the thin film preparation equipments (lase evaporation, magnetron sputtering, and electron beam evaporation), microscopic analysis instruments (including infrared spectrometer, fluorescence spectrometer, step profiler, metalloscope interaction system), and the property measuring equipments for materials and electrons feature testing.

3 THE WORKS IN THIS SPECIAL ISSUE

Professor Chuan-Lu Yang focuses on the theoretical study of ultra-cold molecules. Recently, he and coworkers have calculated the dense potential energy curves of $1^1\Sigma^+$, $1^3\Sigma^+$, $1^1\Pi$, and $1^3\Pi$ states of $LiBe^+$ molecule. The analytical potential energy functions have been constructed with a Morse long-range potential function and nonlinear least squares method. The rotational and vibrational energy levels of the four states are determined by solving Schr?dinger equation of nuclear movement. The spectroscopic parameters are deduced with the obtained rotational and vibrational energy levels.

Professor Meishan Wang *et al.* investigated the equilibrium structure, spectroscopy constants and anharmonic force field of PO_2^- anion. The computed geometries, rotational constants, vibration-rotation interaction constants, quartic centrifugal distortion constants, and coriolis coupling constants of PO_2^- are compared with the available experimental or theoretical data. The fundamental frequencies, rotational constants of ground state, sextic centrifugal distortion constants, cubic and quartic force constants of PO_2^- are firstly predicted. The results show that the B3P86/6-311++G(3df, 3pd) results are in excellent agreement with experiment and represent a substantial improvement over the results obtained from MP2. The other DFT methods are also advisable choices to study the anharmonic force field of PO_2^-. The predicted spectroscopic constants may provide the useful data for the experiment studies of the corresponding spectroscopic constants of PO_2^-.

Professor Xiaoguang Ma presented a graphic method for studying multi-atom resonant photoemission process in molecules and solids. The Feynman diagrams have been

applied to describe the interactions between atoms in MnO molecules. The theoretical results show that the resonant contribution exhibits a strong distance-independent and element specific effects for the neighboring atoms. Two mechanisms, the interactions between the atoms and the reabsorption process have been supposed in the present work to explain the multi-atomic resonant photoemission for the first time.

Professor Zhi-Hong Zhang and coworkers have studied the stereodynamics of the atom-molecule reaction $N(^4S)+O_2(X^3\Sigma_g^-)\rightarrow O(^3P)+NO(X^2\Pi)$ by quasi-classical trajectory method with the lowest $^2A'$ potential energy surfaces (PESs) given by Sayós *et al.*. They found that the degree of the forward scatting and the product polarizations show obviously change along with the initial vibration number, which leads to the increase of alignment and decrease orientation of product rotational angular momentum. The initial rotational excitation makes the alignment of the product rotational angular momentum small change in a certain range. Moreover, the $P(\theta r)$ distribution and $P(\phi r)$ distribution change noticeably by varying the initial vibration number.

Professor Xiaoming Tan has revised the additivity rule for electron scattering from molecule by considering the difference between the free atom and the corresponding bound atom in the molecule. The total cross sections for electron scattering from plasma etching molecules CF_4, C_2F_4, C_2F_6 and C_3F_8 have been calculated in the energy range from 100 eV to 5000 eV with the revised additivity rule. The present calculations are compared with the original additivity rule results and the existing experimental data. A better agreement between the present results and the experimental data is obtained.

Meishan Wang[†] and Aihua Gao[‡]
School of Physics and Photoelectrical Engineering, Ludong University, Yantai, China.

4 AUTHOR INFORMATION

Notes
[†] M. S. Wang. E-mail: mswang1971@163.com.
[‡]A. H. Gao. E-mail: gao_0328@163.com.

5 ACKNOWLEDGMENTS

We thank the National Natural Science Foundation of China (Nos. 11474142, 11074103), Discipline Construction Fund of Ludong University, the University Science & Technology Planning Program of Shandong Province under Grant No. J13LJ04, Ludong University. Finally, we also thank Professor Keli Han from the Dalian Institute of Chemical Physics of Chinese Academy of Science.