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A Biographical Note Regarding My Academic Path

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Abstract

I engage into the research of theoretical chemistry and condensed physics based on first-principles. My research directions cover a wide range among physics, chemistry, as well as materials science. To list a few representative research interests: 1. molecular spectra; 2. chemical kinetics; 3. molecular excited states; 4. molecular reaction dynamics and 5. engineering alloy design.

Keywords: Physics; Molecular Reaction Dynamics; Theoretical Chemistry; Alloying Effects

During the last few years, I received some invitations for delivering a speech regarding my research work in science. Additionally, there are many concerns about my personal profile both in the internet and in some academic institutions. Therefore, it seems necessary to write a review about my personal experience and my research work in science at this particular time.

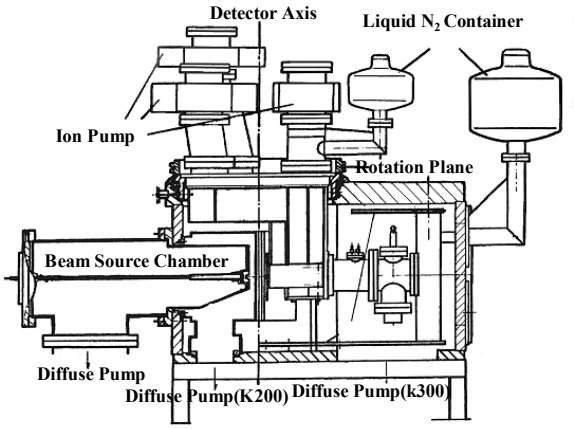
The Research Experience When I Was Major in Physics

I was major in applied physics at Dalian University of Technology (DUT), Department of physics (China) during the time 1999.9-2003.7, and received my bachelor's degree in 2003. Like someone else who studied physics, I learnt theoretical mechanics, electrodynamics. thermodynamics and statistical physics, as well as quantum mechanics in sophomore. In junior and senior, I noticed some research directions or research topics through listening to some reports and speech made by the faculties in the physics department. For example, quark confinement in theoretical physics by one of my teachers, who had taught us quantum physics. The experimental search for free quark has no new findings since the quark model was put forward in the year of 1964. Quark confinement is still the fore-frontier problem in modern physics since the quantum chromodynamics (QCD) cannot prove quark confinement directly. Non-topological soliton model is very successful in describing the static properties of hadrons [1].

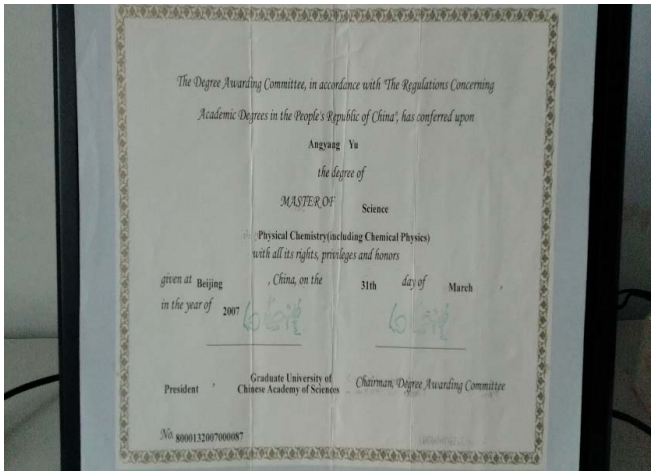
Beginning with the soliton model, a soliton solution has been obtained. The calculated results show that the mass of quark is zero inside hadron, whereas the mass of quark outside the boundary of hadron is much larger than the mass of quark inside hadron. Therefore, much more energy is needed to generate a quark outside hadron than the energy needed to generate a quark inside hadron, which serves as a good explanation of quark confinement [2].

I had also touched upon the field of molecular reaction dynamics through a seminar report made by my senior sister apprentice. Later on, the physics department organized a visit to the State Key Laboratory of molecular reaction dynamics in Dalian Institute of Chemical Physics, where there is the universal crossed molecular beam apparatus as is shown in Figure 1, which gave me a deep impression and set the foundation for writing a review regarding some important experimental techniques in molecular reaction dynamics [3].

This review has introduced some representative crossed molecular beam apparatus in molecular reaction dynamics. A history of crossed molecular beam equipment is reviewed in this paper. The detectors of both the universal crossed molecular beam machine and Hydrogen atom Rydberg tagging apparatus have been discussed. Other types of crossed molecular beam instruments have also been reviewed. Each experimental apparatus makes a compromise among the resolution, sensibility and universality. Hopefully, new types of experimental techniques can emerge and contribute the development of molecular reaction dynamics and relevant research fields.



Universal Crossed Beam Molecular Reaction Dynamics Machine


The Degree Awarding Committee, in accordance with 'The Regulations Concerning Academic Degrees in the People's Republic of China', has conferred upon Angyang Yu the degree of MASTER OF Science in Physical Chemistry(including Chemical Physics) with all its rights, privileges and honors given at Beijing, China, on the 31th day of March in the year of 2007. President, Graduate University of Chinese Academy of Sciences. Chairman, Degree Awarding Committee. No. 80001320070008?

I had learned a course called plasma physics in my junior. Although there are famous advanced Tokomak apparatus in the experiment more attention is paid to the theoretical side, including sheath and positive column [4-7]. Positive column of direct current (DC) glow discharge is primarily used in the field of plasma material surface modification. In this kinetic modeling of a hydrogen glow discharge positive column, electron energy distribution function (EEDF) is found to depart from Maxwell distribution obviously. The distribution tail moves to higher energy when the ratio between electric field E and density of neutral species N (E/N) increases and the tail moves towards higher energy if hydrogen atom proportion increases at the same E/N. It is shown that electronic temperature rises with the increase of E/N. Additionally, the dissociation ratio percentage of H2 augments with the rise of E/N.

My junior and senior were mainly concerned with semiconductor physics. My graduation design is concerned with GaN semiconductor crystal growth using Monte Carlo method. I had written a FORTRAN code to simulate the growth process of GaN crystal. As an important third-generation semiconductor material, GaN can also be investigated by First-principles [8, 9]. During the period of my graduation design, one of my senior fellow apprentices advised me to enter into DICP to perform my research work. With some interests in the chemical reactions at molecular level, namely, molecular reaction dynamics, I entered the examination of national research students after some prior inquires and preparations for the exam and was enrolled by Dalian Institute of Chemical Physics, Chinese Academy of Sciences in 2003.

The Route of Obtaining My Master's Degree

I continued my research work at State Key Laboratory of Molecular Reaction Dynamics, Dalian Institute of Chemical Physics (DICP) and obtained my master's degree in 2006. My diploma at that time has been presented below.

There are two main research interests for me from 2003.9 to 2006.7. The former is the calculations of molecular spectra using quantum physics method. A modified three-dimensional discrete variable representation (MDVR3D) program which could be used to calculate the bound states vibration spectrum of some tri-atomic molecules is developed [10,11]. Both the three-dimensional discrete variable representation (DVR3D) program and the MDVR3D program are used to calculate the vibration energy levels of the isotopic species of hydrogen sulfide ($H_2{}^{32}S$, $H_2{}^{33}S$, $H_2{}^{34}S$, $D_2{}^{32}S$, $D_2{}^{33}S$, $D_2{}^{34}S$, $T_2{}^{32}S$, $T_2{}^{33}S$, $T_2{}^{34}S$). This work forms the basis for dealing with the rotational spectrum calculations and presents the first theoretical results for $D_2{}^{33}S$, $T_2{}^{32}S$, $T_2{}^{33}S$ and $T_2{}^{34}S$.

The latter is the investigation of molecular reaction dynamics using classical trajectory method. The quasi-classical trajectory (QCT) calculation for the reaction O(1D) +CH4 was performed based on a new London-Eyring-Polanyi-Sato (LEPS) potential energy surface (PES). Attention of this work has been attached to the OH+CH3 product channel. Product angular distribution has been studied, which are in excellent agreement with previous experimental results. It is found that there is a forward scattered peak and a backward scattered peak for the OH product relative to the O(1D) beam direction at the collision energy of 6.8Kcal/mol [12].

The Research When I Was Serving as A Teaching Faculty in Liaoning University of Petroleum and Chemical Technology

After graduation from DICP, I worked as a teaching faculty in Liaoning University of Petroleum and Chemical Technology (LNPU) between the year of 2006 and 2011, when scientific research was still an important part of my daily work as the college attaches particular importance to published papers in all kinds of scientific journals. My first published work in this university is a review regarding the geometric phase effect [13]. Some theoretical approaches, including the geometric phase effect, were reviewed because there are many breakthroughs and progresses about the theory of conical intersection in the past years. Some results concerned with the geometric phase effect in the reaction dynamics had been demonstrated and there were also explana-

tions for those intriguing results in this review. It is known that conical intersection could influence nuclear dynamics through the geometric phase effects. The Schrodinger equation acquires a vector potential term in the adiabatic representation. Based upon this expression and the theoretical treatment of the nuclear Schrodinger equation in the diabatic representation, a new equation is derived which incorporates both the geometric phase effects and other non-adiabatic factors [14].

As a teaching faculty in LNPU, I had taught some college experiments to the Freshman and sophomore, for example, the resistance measurement by Wheatstone bridge. In view of its importance in measuring resistance, Wheatstone bridge has played an important role in resistance measurement. My work aims to improve the measured accuracy and precision of self-organized bridge and box bridge, as is shown in the figure below, with the left denoting the box bridge and the right standing for the self-organized bridge.

The experimental results obtained thus far have reached an unprecedented high level for high-precision measurement. To the largest extent for a specific resistance, both the self-organized bridge and box bridge have gained the most consistent measured value [15].

The research when I worked for my Doctor's degree

During the period 2011.8-2014.7, I performed my research work at Institute of Theoretical Chemistry, Jilin university, Changchun, Jilin province, and obtained my PhD's. degree in 2014 at Jilin University of China.

The Main Research Work During This Time Can Be Summarized as Follows:

4.1 The Investigations of Chemical Reaction Dynamics of Elementary Chemical Reactions

It is well-known that controlling the chemical reactions of atmospheric pollutants is a feasible way to solve the environmental pollution. These atmospheric pollutants are mainly produced from radical-molecule or radical-radical reactions. Since these types of reactions are fast and complicated in the microscopic level, it is very difficult to measure experimentally. Therefore, theoretical chemistry methods are needed to investigated this type of reaction. Based on the computed potential energy surface, it is feasible to predict the possible reaction products and best reaction channel, as well as the dependence of reaction rate constants with temperature. Additionally, the calculation of reaction products' ratio in atmosphere chemistry and combustion can serve as a theoretical guide for future experimental research [16-18].

4.2 The Quest for Molecular Properties in Excited States

The ground and low-lying excited states of some organic molecules have been studied theoretically. The calculated vertical excitation energies and vertical ionization potentials are compared with available experimental values. In addition, the vertical electron affinity and the adiabatic electron affinity are calculated either [19-22].

4.3 Stability and Aromaticity of New Super-Atomic Compounds [23].

As some applications in the related field of chemical and material science, this work aims to presentate and characterize some new chemical materials. A new series of compounds Al3-X (X=F, LiF2, BeF3, BF4), consisting of aluminum trimer and fluorine atom or its superhalogens (LiF2, BeF3, BF4), have been theoretically designed. The best interaction orientation between Al3 cluster and fluorine atom or its superhalogens (LiF2, BeF3, BF4) has been identified and binding energies of this type of compounds have also been calculated. HOMO-LUMO energy gap of these compounds has been used to test the stability of these compounds. Additionally, aromaticity of this type of compounds has been confirmed.

5. Postdoc Position at Institute of Metal Research, Chinese Academy of Sciences

After obtaining my Ph.D. degree at Jilin University in China, I was awarded a Postdoctor's Fellowship to investigate titanium alloys' oxidation at Institute of Metal Research, Chinese Academy of Sciences from 2014.12 to 2016.06. My Postdoctor's research performed in Chinese Academy of Sciences can be listed as follows.

5.1 Effects of Alloying Elements on Ti/TiO2 interface

First-principles method has been successfully applied in the condensed state physics. The first-principles method is used to find out the oxidation properties of titanium alloys. Since the simulation is at the atomic level, it is possible to find out some clues of improving the oxidation resistance of titanium alloys [24, 25].

5.2 Computation of Stacking Fault Energy in Titanium Alloys

In the realm of materials science, the research of plastic deformation of metals attaches great importance to stacking fault energy (SFE). In this paper, we derive the expressions of four types (I1, I2, E and T2) of basal plane SFEs of hcp-Ti within the framework of the Ising model. Based on this model, alloying effects on the stacking fault energy (SFE) of titanium alloys are investigated via first-principles calculations. It is found that SFE always decreases with addition of alloying elements.

The distribution of lattice parameters of all the studied Ti95X5 has a direct relationship with alloying element's atomic radii. Additionally, SFEs decrease linearly with the solute's concentration increasing in the Ti-based alloys. This work provides some useful data for new Ti alloys design [26].

5.3 Insights into Structure, Electronic and Mechanical Properties of RuBx (x=1, 2, 3)

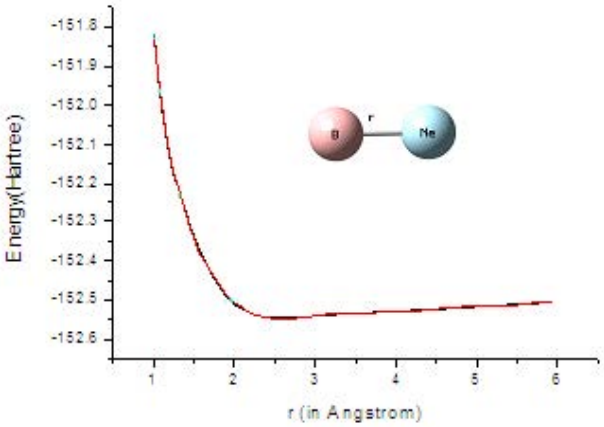
My original research dream in materials science is related with mechanics of materials. In the computational materials studies during my postdoctoral period, the structural, electronic and mechanical properties of RuBx(x=1,2,3) are investigated by performing first principles calculations using density functional theory (DFT). The calculated lattice constants agree well with the available results. The chemical bonding is interpreted by calculating the electron localization function (ELF). The covalent Ru-B bond and B-B bond become stronger with the increase of boron's concentrations, which can help improve the hardness of RuBx system. Moreover, RuB has the highest bulk modulus, which means more prominent volume-compression resistance. RuB2 has a certain elastic anisotropy and RuB3 has the best toughness [27].

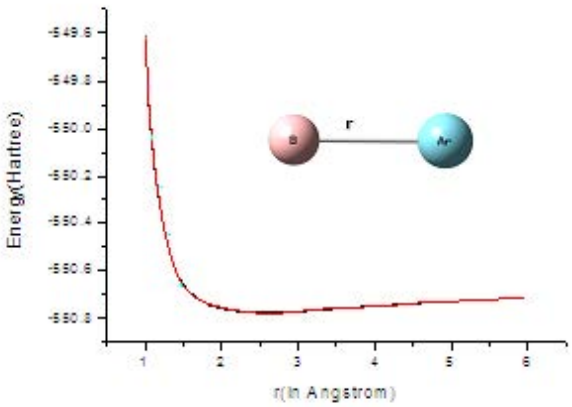
6. Visiting Scholar, Ludong University (2016.10-2018.11)

My research work had been guided by many eminent professors, who gave inspirations in my research. I had acted as a Visiting Scholar from 2016.10 to 2018.11 in Ludong University, where I performed some scientific research work in molecular physics and physical chemistry. Some topics are listed below:

6.1 The Potential Energy Curves and Spectroscopic Constants of the Diatomic BX (X=He, Ne, Ar, Kr)

It is well-known that the Configuration self-consistent field (MCSCF) method is most suitable for the calculation of the potential energy curves or potential energy surfaces. In this work, this method is adopted for the investigation of 4Σ- state in the diatomic BX (X=He, Ne, Ar, Kr), as is exhibited in those figures below. The computed energies of potential energy curves (PEC) for the B-X (X=He, Ne, Ar, Kr) series are fitted to analytical potential energy function (APEF) using nine-order Murrell-Sorbie function. Compared with previous results, more accurate spectroscopic constants have been obtained. To describe the dissociation behavior correctly, the dissociation energy and equilibrium distance of the B-X (X=He, Ne, Ar, Kr) series have also been determined. Additionally, some vibration energy levels of this electronic state have been predicted, and they are in excellent agreement with experimental data.





6.2 Partial Potential Energy Surfaces and Their Application to Reaction Resonances

Feshbach resonances do not restricted to small reactive systems such as $F+H_2$ and IHI [28]. It can be found in many reactive systems. In this work, the concept of the partial potential energy surface (PPES) is introduced. It is shown that the dynamic Eyring lake explains very well the existence of reactive resonances in elementary chemical reactions. Particularly, the PPESs of the $Cl+CH_3CH_2Br$ and $Cl+CH_3CH_2CH_2Br$ systems including the minimum energy path (MEP) and the vibration potential energy curves were constructed using quantum chemistry methods. Based on the constructed PPESs, the scattering resonance states of these reactions can be expected and the resonance state lifetime was estimated [29].

7. My Recent Research Work

Substitution effects are common phenomena in natural science. To a large extent, substitution of methane with chlorine will influence the mechanism and kinetics of the reactions between chloromethane and atomic chlorine [30]. In the area of molecular spectra, vibration energy levels of hydrogen sulfide substituted by isotopic elements will shift [11]. Additionally, alloying element's substitution in titanium alloy can improve oxidation resistance in the realm of material sciences [24, 25].

In my recent work, the geometry, electronic structure, and infrared spectra (IR) of meso-tetra-substituted porphyrin have been investigated. The substitution of pyridyl for phenyl in meso-tetra-substituted porphyrins can result into the reduction of molecular size, including the molecular diameter, as well as the size of the central ring of porphin. It has also been found that the molecular orbital energies of T3PyP are smaller than the counterparts of TPP whereas there is almost no change in the HOMO–LOMO gap. Additionally, the infrared spectrum of TPP and T3PyP has been compared in order to determine whether there is a red shift or a blue shift [31].

In recent days, I also reflect upon the source of innovation and the art of discovery in physics[32], simply because many breakthroughs in the history of physics originate from the raising of scientific questions and promote the true progress of science and technology. Physicists not only have the courage to innovate and face difficulties, but also can use the correct research methods to show the art of scientific discovery to the world.

8. Concluding Remarks

My research experience dates from the year of 2003, when I was performing my graduation design in Dalian University of Technology (DUT). As the first author or corresponding author, I have published more than 30 scientific articles in many international journals. The intention of this article is not only to introduce my personal experience, but also to explain my research profiles during the past several years. The topics of my research belong to physical chemistry and chemical physics.

Acknowledgement: I want to express my thanks to my parents, my relatives and my friends for putting up with me.

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