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## Molecules during Stellar Formation and Death

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# Publications

## Refereed publications

My major publications are listed as follows, among which the latest three (items 1, 2, and 3) are my favourite papers.

In item 3, accurate  $N_2$  photodissociation rate and shielding functions were calculated. The results are very useful in many astrophysical fields. Both chemists and astronomers worked hard for this aim for decades. In item 2, a new method for accurately calculating molecular shielding functions in full 3D radiation field was proposed, and was employed to give new predictions for molecule distributions in a C-rich AGB star, IRC +10216. In item 1, a detailed discussion on the chemistry in O-rich AGB stars was carefully conducted based on the latest progress from both observations and simulations. By far, the results are the most accurate ones, and can be directly compared to the future observations.

1. **Xiaohu Li**, Tom J. Millar, Alan N. Heays, Catherine Walsh, Ewine F. van Dishoeck, and Isabelle Cherchneff, *The chemistry and distribution of daughter species in the circumstellar envelopes of O-rich AGB stars*, Submitted to A&A, 2015 (18 pages, Impact factor 5.084)

2. **Xiaohu Li**, Tom J. Millar, Catherine Walsh, Alan N. Heays, and Ewine F. van Dishoeck, *Photodissociation and chemistry of  $N_2$  in the circumstellar envelope of carbon-rich AGB stars*, A&A, 2014, 568, A111 (13 pages, Impact factor 5.084, citation: 1)

3. **Xiaohu Li**, Alan N. Heays, Wim Ubachs, Brenton R. Lewis, Ruud Visser, and Ewine F. van Dishoeck, *Photodissociation of interstellar  $N_2$* , A&A, 2013, 555, A14 (18 pages, citation: 9, Impact factor 5.084)

4. **Xiaohu Li**, Ewine F. van Dishoeck, Marc C. van Hemert, and Carina Arasa, *Effects of reagent rotation and vibration on  $H + OH(v, j) \rightarrow O + H_2$* , JPC-A, 2013, 117, 12889 (8 pages, Impact factor 2.775, citation 1)

5. **Xiaohu Li**, Meishan Wang, Ilaria Pino, Chuanlu Yang, and Lingzhi Ma, *The stereodynamics of the two reactions:  $H + LiH^+(v=0, j=0) \rightarrow H_2 + Li^+$  and  $H^+ + LiH(v=0, j=0) \rightarrow H_2^+ + Li$* , Phys. Chem. Chem. Phys., 2009, 11, 10438 (8 pages, Impact factor 4.198, citation: 39)

6. **Xiaohu Li**, Meishan Wang, Ilaria Pino, Chuanlu Yang, and Jicheng Wu, *The isotopic effects on stereodynamics for the two reactions:  $H + LiH^+(v=0, j=0) \rightarrow H_2 + Li^+$  and  $H^+ + LiH(v=0, j=0) \rightarrow H_2^+ + Li$* , Phys. Chem. Chem. Phys., 2010, 12, 7942 (8 pages, Impact factor 4.198, citation: 9)

7. **Xiaohu Li**, Meishan Wang, Chuanlu Yang, Lingzhi Ma, Ning Ma, and Jicheng Wu, *The polarization dependent differential cross sections of the reactions:  $H + LiH^+(v=0, j=0) \rightarrow H_2 + Li^+$  and  $H^+ + LiH(v=0, j=0) \rightarrow H_2^+ + Li$* , Chin. Chem. Lett. 2010, 21, 376

8. Jicheng Wu, Meishan Wang, Chuanlu Yang, **Xiaohu Li**, and Xiaoqiong Chen, *Theoretical Study of the Stereodynamics of the Reaction  $C(^3P) + CH(X^2\Pi)$  and Its Isotopic Variants*, Chin. Phys. Lett., 2011, 28, 063401
9. Lingzhi Ma, Meishan Wang, Chuanlu Yang, Chunyan Xia, **Xiaohu Li**, and Ning Ma, *Influence of reagent rotation on the integral cross sections of the collision  $(He, HD^+)$* , J. At. Mol. Phys., 2009, 26, 3
10. Lingzhi Ma, Meishan Wang, Chuanlu Yang, Chunyan Xia, and **Xiaohu Li**, *The Stereodynamics Study on the Reactions of  $He + H_2^+(HD^+, DH^+)$* , Ludong University Journal (Natural Science Edition), 2008, 4, 13
11. Ning Ma, Meishan Wang, Chuanlu Yang, Xiongde Lin, **Xiaohu Li**, and Xiaoguang Ma, *Theoretical study of the influence of laser intensity on the population of the NO molecule electronic states*, Acta Phys. Sin., 2010, 59, 251

## Conference proceedings

1. **Xiaohu Li**, Ewine F. van Dishoeck, Marc C. van Hemert, and Carina Arasa, *Effects of reagent rotation and vibration on  $H + OH(v, j) \rightarrow O + H_2$* , The Molecular Universe, Posters from the proceedings of the 280th Symposium of the International Astronomical Union held in Toledo, Spain, May 30-June 3, 2011.

## Curriculum vitae

I was born in the center of Jingning County, Pingliang city, Gansu Province, the People's Republic of China. There are quite a few interesting places there. For instance, 3 km away from my home, there is a small library together with the majestic Fu Xi Temple. Fu Xi is one of the cultural heroes in Chinese legend and mythology, and he is thought to be the "original human". In particular, it is said that he created the *BaGua*, which are eight trigrams used in *Taoist* cosmology. Importantly, the *BaGua* consists of only two fundamental elements: *Yin* and *Yang*, which are also the basis of *Taichi* ("Supreme Ultimate" state). The *BaGua* and *Taichi* may represent the best wisdom of Chinese philosophy over its long history.

Here is a simple route of my education. My first school was the No. 1 Kindergarten in Jingning. There I did very well and got my current name, Xiaohu, which means 'small tiger'. I got this name because my teacher told my father that I looked like a lovely little tiger. Two years later, I was sent to a primary school. At the beginning, I refused to go to that school, because the teachers there always gave lots of home work. After an impressive beat from my mother, I finally agreed to take classes and eventually became the top student. Then I entered into middle school. Quickly, I became the class leader in my class, and had some other 'important' tasks as a student leader. I obtained the best scores and also helped some other students to make progress. Afterwards, I entered into the best middle school, called "No. 1 middle school" in my county, where I met some 'genius' and we became very good friends. After the graduation, we took a terrible exam, called 'Gao Kao', which is the entrance examination to the university. Unfortunately, I did not make a good score, which made me spent my next 4 years in Hexi university.

The good thing was that I was in the physics department. Again, I became the students leader and organized lots of student activities. I built the first 'English Corner' for the physics department, and invited many foreigner teachers to tell us something about their countries and culture. After I got my Bachelor degree, I passed the entrance examination of a 3-year master program of Ludong University, and my research was fully financed. In the very beautiful seaside city, Yantai, I started my master studies under the supervision of Prof. Meishan Wang. Quickly, I became the class leader in my class, though there were only 6 students in total, and we were divided into 3 different fields, including pure theory, numerical simulations, and experiments. My research topic was atomic and molecular physics, specifically working on molecular reactions. Because we were only 6 classmates, to make our teachers feel better, all of us attended all of the courses in three different fields, and took the examinations. An important thing for my life was that I met Miss Changchun Song in that university, and quickly, she became my girlfriend. One and a half years later, she became my wife, and now, she is still my wife.

After I got my master degree with the best record in Ludong University, I went to Dalian Institute of Chemical Physics (DICP), Chinese Academy of Science, work as a staff member in Prof. Keli Han's group. I would say that DICP is the best chemical-physics institution in China. One of my idols, Prof. Can Li, is also working there. There I learnt basic techniques and theory about experiments on femtosecond ultrafast dynamics from Prof. Jianyong Liu. By that time I only had a master degree, to get a better position I must obtain a PhD degree, either at DICP or other places. I had a few options. Suddenly, I noticed that Prof. Ewine van Dishoeck was looking for a PhD student. After a Skype interview, I got the position quickly, within 2 hours. Before coming to Leiden, I did not take any astronomy courses. But two years later, when I

started to do a project on astrochemistry, I started to step into this field very quickly, partly because the project was much more interesting than any other projects that I have ever done before, and partly because I had no time to wait. So, ‘quickly’, is a good word during my study. Nowadays, it becomes important to determine things fast and take actions.

A few more words about my life and study in Leiden, a university city since 1575. Leiden is a small, quiet, beautiful, friendly, and very interesting city, but looks quite modern, especially Leiden Observatory where I have been working/studying for 4 years. Here, I met and talked with many very nice, smart, and distinguished people. I attended a lot of interesting and impressive conferences, including most of the astrochemistry seminars and theoretical chemistry group-meetings organized by the Astrochemistry Group in Leiden Observatory and the Institute of Theoretical Chemistry of Leiden University. I selectively attended some of the Sterrewacht Colloquia, “This week’s discoveries”, and especially some workshops held in the Lorentz Center. I gave talks or presented posters at a number of international meetings, e.g., IAU280 “The Molecular Universe” Symposium in Toledo (Spain, 2011), the annual Dutch Astrochemistry Network (DAN) network meetings, NOVA Network II meetings, Faraday Discussion 168 meeting (2014, Leiden), etc. In particular, I was selected to attend the Onsala Space Observatory summer school “Molecules in space”, with applications from PhD students and postdoctoral researchers all over the world with only 15% chance of success. There I made my first real observations towards the molecular cloud CB 17 using the Onsala 20m mm-telescope, and my report achieved the top score.

I got many honours and awards during my 26 years of studies, mostly due to helping other students, organizing student activities, and hard-work, sometimes due to competitions. Eventually I understood that it is not important how excellent/distinguished a person is, but that it is important to what extent one can help/influence other people. Contributions and mercy are very important to be a good scientist. Meanwhile, life is short, and sometimes life is hard to many people. I mention this here because one of my very good friends, one of my ‘genius’ classmates during my middle school, died in May of 2014 in Beijing, partly due to lots of hard work. Moreover, some other ‘successful’ people have died at a very young age. Therefore, enjoying one’s own work, having fun, and being happy are much more important than so-called ‘success’. Good attitudes are very important to human beings, including scientists.

I would like to close this section with an interesting story of my own. In China, there was a very traditional question: what do you want to be when you grow up? Many of my classmates wanted to be a teacher, a policeman, an engineer, a scientist, etc. And many of them forgot their original aims when they grew up. My answer to that question was, “I want to be an Astronaut” (I was like 8 years old at that time), and I also forgot my words for a long time. When I started to write this section, suddenly I realized that now I am very closing to my original dream: rather than an “Astronaut”, I am on my way to be an “Astronomer”, which suits me even better. Just like an interesting saying, “Everybody should have a dream, what if that dream comes true?!”.

# Acknowledgements

IT is not easy to obtain a PhD degree, which is probably one of the reasons why most PhD students want one. So, we came, we conquered, and we gained. The degree is useful, but what is more important is how we got there and what we learnt during this process. Meanwhile, the “new” faces we meet and communicated with, together with the “old” faces that always exist in our memory can give us power to move forward, overcome difficulties, feel love, feel friendship, remember our responsibilities, and motivate us to do our best to perform better and better. Because of them, we always cherish our good luck and appreciate the beauty of this planet, and in turn try to help others and make the world a little bit better. These people include our families, friends, teachers, collaborators, students, and also some distinguished opponents. It is hard to mention all of them here, but never mind, I don't really wish to, and couldn't fully express the thanks from the bottom of my heart with words. Instead, I will always remember the good times we spent together and try to keep in touch if it is possible. I will miss them. These memories are mine and will stay with me forever. So, just a few sentences and a simple list of the names for those people I can remember at the moment.

According to Leiden tradition, Leiden professors are not acknowledged in this section. I appreciate the spirit but I must mention that we have quite a few very distinguished professors at Leiden University, especially in the Leiden Observatory. Many of our professors are very well-known in the world. To some extent it is really these professors who work very hard day-by-day and continue the glory of the University, and benefit the students generation-by-generation. Any small piece of work from us students contains lots of contributions from our supervisors, in addition to valuable discussions with other professors during various seminars, a simple drop by, lunch, or any other connection. Some of these professors are my very good friends, shared me with their knowledge, wisdom, favourite music, poems, interesting stories, ‘paper cakes’, cookies, and delicious home-made food. So, my deepest thanks!

Then, a few names that guided me, and closely interacted with me. Alan, my co-promoter plus brother, it is so great to have you involved in all of my projects, you are such a nice, helpful, patient, and considerate guy! Carina, a very nice person who, always smiles and very patiently, taught me quite a few things, even including how to make movies of molecular reactions. Ruud, you taught me my first astrochemical modeling, and then continued to help me with various details. Catherine, one of my office mates, trained me with dark cloud models and then brought me into my favourite field, AGB envelopes. Well, a big name, Tom Millar! Every time I meet you, including the first time, made me feel very happy. You shared with me your wisdom, many stories, and hosted me with very delicious food every summer during my visit to your group in Queen's University Belfast in the past two years. Our friendship will last forever. Lars, I cannot appreciate your spirit too much, I miss the time when you were in our office. You are the person I can always rely on. Jiancheng, Dongfeng, Junfeng, Feijia, and Ko-ju, only with you can I discuss the scientific questions in another language, it is such a pleasure to meet you guys here! Oh wait, also with Gleb, a smart guy who can even play Chinese chess and Pingpang with me! Our very international astrochemistry group members, we spent many Friday mornings together, shared ideas, discussed progress, learnt from the same materials, celebrated many achievements, in addition to preparing talks and posters for many international conferences. We had lots of parties together, including our annual retreats, with various nice dinners. We are belonging to a special “family”, lead by our “Queen”. I will miss you guys soon, especially the first Friday

after I leave Leiden. OK, no more words are needed, I believe you guys understand that I cannot express the feeling, no matter how hard I try. So, just list your names: Lars, Ruud, Isa, Jeanette, Carina, Geoff, Catherine, Mihkel, Anna, Alan, Umut, Daniel, Agata, Magnus, Joe, Irene, Nienke, Kenji, Niels, Maria, Paola, Simon, Davide, Nadia, Christian, John, Andreas, and Vianney. In the past 4 years, I am staying in one office, 503. My office mates used to be Lars, Jeanette, Remco, Geoff, Jaya; Currently, are: Mihkel, Anna, and Catherine. Basically, everyone comes from a different country, but the daily greetings, the funny chat, the smile/laughing, the care, the help, the warm words, and understanding, are the same. I remember many of you guys' favourite sayings and words, e.g., "Yes and No!", "Think differently!", "Don't be childish, stick to our plan!", etc., also "Could be better, could be worse" . You guys are so smart, funny, and considerable! It was/is my great pleasure to be your office mate, wish you every success and good luck in the future!

A special thanks goes to Nienke. Not only because you translated the Dutch summary for my thesis during the New Year holiday time, but more importantly, during my 4 years of living in your country, whenever I needed your help you were always there. You are among one of the most lucky Ph.D. students since your first first-author paper has been published in Science.

The computer staff, Erik, David, Aart, and Niels, in addition to secretaries, Liesbeth, Anita, and Jacqueline, amongst others in our department, and at the Graduate School, are just excellent and very efficient. Without any of your help the process of this thesis would take a much longer time. I am also very grateful to Evelijn Gerstel and Eveline Castermans for lots of kind help and support.

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At Leiden Observatory, some of my colleagues and friends were not directly involved in my scientific work, but shared with me friendships, in particular, Carl, Daniel Caputo, Sergio, Mateo, Emanuele, Francisco, Daniel Paardekooper, Leen, Heather, Michiko Fuji, Steven, Shuro, Edith, Anton, Nicola, Olmo, Silvia, Olivera, Steven, Kalle, Rafael, Kuo-Song, Thanja, David, Pablo, Edwin, Sebastiaan, Carmen, Marissa, Tiffany, Gilles, Berenice, Alexander, Marco, Alessandra, Grainne, Jean-Baptiste, Tim, Luke, Silvia, Markus, Isabel, and Pamela. Sascha, Alex, and Josha, you three gave me and my visitors tours to the old observatories, introduced the history and telescopes there to us, and guided us to observe the beautiful stars. I still remember the feeling of sitting on Albert Einstein's favourite chair, and the exciting moment when I saw a clear surface of the Moon, the Jupiter with moons, also Saturn, Titan, and Mars. Wish you all the best in the future and good luck for your thesis! Surprisingly and happily, I met an excellent Pingpang opponent here- Walter Jaffe, who used to be a member in a Pingpang club for more than 10 years. Walter, let's cheers for our friendship and wish you and Lexa every happiness!

I would like to acknowledge the friendship from my friends in the Netherlands outside my working place as well. Qiang Ge and Da Jie, together with Shushu, Ayi, Jiawen and Jiacheng, you like my families. We celebrated many important events together, including every New Year during the past four years. I do believe the Chinese restaurant (Kwangtung Restaurant) you run is the best one in Leiden. Leo and Majella, I will miss you, wish you every happiness. Victory, Fumi, and Clara, thanks for visiting me twice from Taiwan. It is hard to mention everything, so, a list of the names that I can immediately remember: cr; Pq; Fastq; Liang Zhang, Xinyi, Lei Song, Mingli, Xiaoshuang, Shengfa, Yuli, Wen Pan, Changsheng, Chengjun, Jianqiang, Qiang Wang,

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Last but not the least, thanks to my friends that I forgot to mention here, and thanks to the Netherlands Organisation for Scientific Research (NWO) for financing my research!





From left: Xiaohu, Nadia, Kenji, Agata, Irene, Andreas, Ewine, Joe, Anna, Daniel, Catherine, Mihkel, Paola, Alan, Maria, Nienke, Magnus, Niels, Davide, Simon, Ko-ju.



*“Two roads diverged in a wood, and I-  
I took the one less travelled by,  
And that has made all the difference.”*

— Robert Frost









