

BULLETIN OF THE KOREAN CHEMICAL SOCIETY

A Tribute to Professor Kook Joe Shin by Mino Yang[†] and Hyojoon Kim[‡]



Professor Kook Joe Shin

It is with great pleasure that we write this tribute honoring Professor Kook Joe Shin on his retirement from Seoul National University after more than 30 years of service as a faculty member of Department of Chemistry. This special issue of *Bulletin of the Korean Chemical Society* is to celebrate his life-long contributions to the Korean chemistry community, especially in the field of theoretical chemistry. It is also an opportunity for us to express our gratitude for his devotion and passion for educating young chemists in Korea.

His graduate work with Professor Byung Chan Eu, a theorist at McGill University, was to develop a linear response theory for the nuclear magnetic relaxation and the mechanical energy relaxation of methyl group-containing polymers at low temperature. During his postdoctoral studies with Professor Raymond Kapral at the University of Toronto, he developed a microscopic kinetic theory for chemical reactions. The theory was based on the most fundamental equation of motion at the level of classical mechanics, the Liouville equation for hard spheres. As far as we know, this work is the first ambitious effort to apply the kinetic theory formulated for the “simple” dynamics of liquids to the rate theory of chemical reactions in liquids. Considering that most of the rate theories for liquid reactions had been formulated with phenomenological diffusion equation, his work using the microscopic equation of motion may be appreciated as an approach that science should ultimately pursue.

After spending two years in Toronto, he joined Seoul National University as a faculty member of Department of Chemistry. Since then, his research has been focused on understanding various dynamical phenomena occurring in condensed phase, particularly in liquid phase, such as molecular rotational diffusion, kinetics of nonlinear chemical reactions, molecular diffusion on solid surfaces, and rate theory of diffusion-influenced chemical reactions. For this, analytical methods for theoretical formulation as well as computer simulation methods such as molecular dynamics and Monte Carlo method have been used.

During the 1990's, he collaborated with his students to produce a series of remarkable results on the rate theory of diffusion-influenced reversible reactions which originated from his earlier kinetic theory. During this period, many researchers including S. Lee, A. Szabo, W. Naumann, A. Molski, A. Burshtein, N. Agmon, M. Tachiya, and A. Doktorov were intensively studying the effects of many particles on reversible diffusion-influenced reactions. The kinetic theory approach developed by the research group of Professor Shin was very powerful in describing the complicated competition effects arising from many-body dynamics, and it is still known to be one of the most accurate theories of this field developed up to this day.

In addition to his contributions to the field of theoretical chemistry, he has had a great impact on the education of Korean chemists, including many of the authors contributed to this special issue who have learned Statistical Mechanics through his graduate lectures. He has always been a great teacher for chemistry students and a generous and supportive mentor to his graduate students, allowing them to explore new areas of science under their own motivation, while at the same time providing them with appropriate guidance and encouragement. He has also devoted himself to nourish Korean chemistry community by serving as organizers of many chemistry-related symposia and conferences including “The 3rd International Workshop on Diffusion-Assisted Reactions (DAR)”. As the President of the Korean Chemical Society in 2005, he also showed his strong leadership which positively impacted the Society.

We will miss Professor Shin's crucial scientific contributions, educational efforts and supports to the Korean chemistry community. On behalf of all of his friends and colleagues, we wish him all the best in the future. We thank the Editorial Boards and authors of the articles who have made this special issue possible. We are very pleased to have the honor to serve as Guest Editors for this special issue and to write this Tribute.

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Kook-Joe Shin Retiring

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Life is irreversible, although all underlying chemical reactions are reversible. Thus if two molecules, S and A, meet to form a product SA, this product can later dissociate to reform the initial state:



The simplest case is when only one molecule of type S and one molecule of type A exist. These can meet and separate many times before eventually separating forever. In solution, S and A behave like random walkers, moving around diffusively. This is the geminate limit of reversible diffusion influenced reactions on which we have been working for many years. We were able to find an exact expression for the probability of observing the bound state, SA, but what is the general solution? In a seminal paper,¹ Hyojoon Kim (now a professor in Busan) and Kook Joe Shin showed that the corresponding diffusion equation can be solved analytically for any initial or final state. This has initiated our first encounter.

At that time I was working (with Irina Gopich, now at NIH) on solving the geminate problem when S and SA are in their excited electronic states, applying it to excited-state proton transfer. Prof. Shin got excited, suggesting they can obtain the general solution for this problem as well. I wrote him that Irina was already working on it. His reaction was of rare generosity, proposing that Irina & I publish these results alone.² Instead, he said, we could publish together the solution of the same problem in one dimension. This was our first joint publication.³ It was soon followed by three others: The first two with Hyojoon Kim and the last two with Soohyung Park.

The reader must have perceived by now that the chemical reaction is just a metaphor. In reality



They were driven together by the genuine excitement of S about science.

I first met Kook Joe Shin in the Workshop on Diffusion Assisted Reactions (DAR) that Anatoly Burshtein has organized in the Weizmann Institute (March 14-19, 1999). After the symposium, I travelled back to Jerusalem with two guests, Kook Joe Shin and Sangyoub Lee. On Friday morning there was nobody in the department except us, when Shin and Lee gave a detailed description of their intricate theories for solving the much more difficult many particle case for this reaction.

Our next meeting was in the second DAR conference that Kook Joe Shin, with Sangyoub Lee and Seokmin Shin, have organized in Seoul (Aug. 4-9, 2002). Our lectures were back to back on a Thursday morning, and on a similar topic: Brownian dynamics simulations of many body effects in the $S + A \leftrightarrow SA$ reaction. This conference was memorable for its high scientific level, the many excellent scientists who have participated and, particularly, for the genuine Korean

hospitality.

There was an unforgettable Korean restaurant the night before the conference, with an endless procession of traditional dishes. There was an excursion to the Korean Folk Village, gallantly led by Kook Joe in pouring rain. On the way back the Han River was overflowing, and we barely made it back to the Faculty House. After the conference we decided to take a break from science, when Kook-Joe drove us to Hwaseong Fortress, an 18th century capital on the UNESCO World Heritage list.

Towards the end of 2003, Kook Joe has sent one of his Ph.D. students, Soohyung Park, to visit me Jerusalem. Soohyung has extended our previous work to the reversible ABCD reaction, when the two molecules that react produce two other molecules. Two joint papers emerged from this short visit.^{5,6} In the summer of 2004 S & A met again, this time in the 3rd DAR workshop (organized by Guenter Grampp and Gonzalo Angulo near Leibnitz, Austria).

After completing his Ph.D. work with Kook Joe in 2006, Soohyung returned to Jerusalem as a post-doctoral fellow. Two of the 4 papers that came out of this period dealt with diffusion influenced Michaelis-Menten kinetics of enzymatic reactions,^{7,8} a topic that Kook Joe started investigating in 2001.⁹ A paper by Zhou & Szabo in this issue further discusses this problem.

In 2005 Kook Joe has become the deputy and subsequently the head of the Korean Chemical Society. We have not met again since. But, I believe, after a life full of achievements Kook Joe deserves a rest. Enjoy your retirement!

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Kook Joe Shin, An Excellent Scientist, Teacher, and Administer

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I remember very well the day on which I met Kook Joe in 1994 for the first time. At that time I was the director of division of physical chemistry of our institute. When our institute had distinguished visitors who wanted to see the institute, the office of director-general used to ask one of the division directors to show them to his division. One day I was asked by the office of director-general to show a Korean delegate to my division. This delegate was a group of chemistry professors of Seoul National University. I knew Kook Joe very well by his name, but had never met him. So it was a great surprise for me to find him among the delegate. Later I knew from a message given by him on the occasion of my retirement that when he visited Japan to attend Tokyo-Seoul University Chemistry Conference, he asked the organizer of the Conference to arrange a meeting with me after the Conference.

In 1997 I started a 10-year-term big project as the project leader to make our institute a center of excellence in the field of photoreaction control and photofunctional materials. As a part of this project I organized an international symposium periodically. On the occasion of the third symposium which was held in March, 2000 I invited Kook Joe together with Prof. Rudy Marcus and many other distinguished scientists. Kook Joe gave a nice lecture. I still remember pleasant times I spent discussing science and others with Kook Joe, Rudy, and Guenter Gramp from Technical University of Graz in sushi restaurant, Japanese pub and other places.

In 2001 Kook Joe invited me to Korea. I gave a lecture at Seoul National University. I also gave a talk at Korean Chemical Society meeting which was held in Busan. There was a happening in Busan. Our hotel overbooked, and there was only one room left for two of Kook Joe and me, so the hotel offered a suite as the second room. Kook Joe offered me to take the suite, so I did. This was my first and probably last(?) experience to stay in a suite at such a gorgeous hotel overlooking the sea.

Kook Joe and I share interest in diffusion-influenced

reactions. He pioneered in theory of reversible diffusion-influenced reactions. Last November I met Rudy Marcus in Taipei. On that occasion Rudy asked me about my recent paper on charge recombination in organic solar cells. He also asked me about the works of Kook Joe and Sangyoub Lee on reversible diffusion-influenced reactions. In my guess Rudy is interested in charge recombination in organic solar cells and thinks that the works of Kook Joe and Sangyoub Lee should be important to analyze charge recombination in organic solar cells. I quite agree with Rudy in this respect.

As a meeting in the field of diffusion-influenced reactions there is a meeting titled "International Workshop on Diffusion-Assisted Reactions (DAR)". I think Kook Joe attended all DAR workshops since it started in 1999. I attended DAR workshop twice, first the one organized by Kook Joe in Seoul in 2002, second the one organized by Guenter Grampp in Austria in 2004. In the 2004 workshop I suggested Kook Joe to extend the work he presented. This suggestion developed into our collaboration and we finally published a paper titled "Effect of an External Field on the Diffusion-Influenced Reversible Reaction of a Neutral Particle and a Charged Particle in Three Dimensions" in *J. Chem. Phys.* 29, 234501 (2008) together with his student, Shang Yik Reigh.

In 2005 I met Kook Joe at PACHICHEM which was held in Honolulu by the Chemical Societies in Pacific Basin countries including American Chemical Society, Japanese Chemical Society, Korean Chemical Society and so on. I found Kook Joe attending this conference as the president of Korean Chemical Society. Indeed he deserved it. Kook Joe is not only a good scientist and a good teacher, but also a good administrator. On the occasion of my retirement two years ago he gave me, as a present, a calligraphic writing he wrote for me. He is also an excellent calligraphic writer.

On the occasion of his retirement I thank Kook Joe for his friendship, congratulate him on his successful career, and wish him a good health and a happy second life.

Autobiography

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Throughout my life, I have been fortunate enough to have chances to work with wonderful teachers, mentors, colleagues, and students, who helped my career as a chemist flourish and my view of scientific horizon expand. Especially I have been deeply indebted to my former teachers at Seoul National University, McGill University, and University of Toronto, as well as to my former students at Seoul National University who worked so hard with superb capability and dedication.

I was born on October 19, 1946 in Seoul to my parents, both of whom were scholars; my father, a professor of economics, and my mother, a professor of English literature. During the Korean War, I had to move to a port city of Busan, where I started my elementary school education at a temporary classroom built with military tents and equipped with makeshift benches. After spending long hours for experiments with hand-made wood rocket and vacuum tube radio during my middle and high school years in Seoul, I was admitted to Seoul National University in 1965 where I chose Chemistry as my major on my father's advice that I could learn most up-to-date knowledge in chemistry from young professors U.S. including Professor Taikyue Ree, Father of Chemistry in Korea. Indeed, I got attracted by theoretical aspects of chemistry thanks to Professors Seihun Chang and Hojing Kim who taught me Physical Chemistry, quantum chemistry and statistical thermodynamics.

After three years of military service, I went to McGill University, with my wife, Jeong E. Nam, where I joined the Professor B. C. Eu's theoretical group. After spending a year for torsion pendulum to measure mechanical property of polymer in Adi Eisenburg's polymer laboratory, I finally decided to become a full-time theorist. I applied the linear response theory of John Deutch and Irwin Oppenheim and pressure broadening theory of Ugo Fano not only to the relaxation of mechanical energy but also to the nuclear magnetic relaxation of the internal rotation in polymer at low temperature.

At University of Toronto where I joined Raymond Kapral's group as a research associate, I worked on the generalized kinetic equations taking into account repeated collision events, the generalized Langevin equation, and renormalized kinetic theory of chemical reactions incorporating many-particle effects through the memory function with Robert Cukier and John Mehaffey.

When I came back to Seoul National University in the fall of 1979, it was not at all easy to carry out serious research with a couple of graduate students whose only goals were to

enter American graduate school after their master's degree. Lack of decent archives of scientific journals made the situation worse for research. Nevertheless, I was lucky to have several bright students with whom I was able to work on the theory of molecular reorientation in liquid. We were able to analyze the internal rotation of methyl group in liquid toluene to obtain experimentally verifiable overall reorientation correlation time. Our papers published in *J. Chem. Phys.* and *Chem. Phys. Lett.* in 1982 may be the first ones based on theoretical research carried out in Korea.

When another theorist, Sangyoub Lee, a former student of Martin Karplus, joined our faculty in 1988, it became possible for us to start serious collaborations on diffusion-influenced reactions in solution. Mino Yang was my first Ph.D. student in 1990's, with whom we began to work on the nonlinear chemical reactions and the kinetic theory of chemical reactions in liquid. We were able to find a powerful kinetic theoretical formulation which can be applied to various reversible reactions.

I had wonderful chances to find good friends and coworkers, including Noam Agmon of Hebrew University of Jerusalem and Masanori Tachiya of the National Institute of Advanced Science and Technology in Tsukuba through a series of international symposia on Diffusion Assisted Reactions (DAR) which started at Weizmann Institute of Science in 1999. I was also able to share good friendship with many Russian theorists including Alexander Doktorov (Novosibirsk State Univ.), Alexey Kipriyanov (Novosibirsk State Univ.), Nikita Lukzen (International Tomography Center), and Alexander Ivanov (Volgograd State Univ.).

I should not forget to mention my long-time friendship with Dong J. Lee of Pukyong National University which went back to early 1980's through common research interest in the field of nonlinear chemical reactions. Together we have published 16 very interesting papers, the latest one being on "*Complex oscillations in a simple model for the Briggs-Rauscher reaction*" (*J. Chem. Phys.* 2004). It was also an important accomplishment for me to translate into Korean an excellent popular book "*Order Out of Chaos*" by Ilya Prigogine and Isabelle Stengers in 1988.

I would like to express my deep appreciation to all of my former students and collaborators for teaching and helping me so much that I could achieve what I have done. If any of my research works attracted some attention at all, the major credit should be with them. I would also like to express my deep appreciation to all the authors who contributed their valuable papers to this special issue.