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Preface

From March 31 to April 2, 2014, former students, postdoctoral researchers, collaborators, and colleagues of Jean-Marie André gathered in Beijing to celebrate Jean-Marie's seventieth birthday. I had the honor of organizing an international symposium entitled Quantum Chemistry for Extended Systems, which included a forum for the presentation of recent research. This special issue of *SCIENCE CHINA Chemistry* brings the science that was shared at this symposium to a wider audience.

Jean-Marie was born in a typical Belgian family: his father, Robert, was Wallon whereas his mother, Godelieve, was of Flemish origin. He spent 12 years in a Jesuit school in Charleroi before he entered the Catholic University of Louvain in 1961, where he spent 10 years receiving scientific training. Jean-Marie's graduate work with Prof. George Leroy, which was focused on the electronic structure of polymers, employed a solid-state physics approach that included both Hückel and Pariser-Parr-Pople Hamiltonians, well before the 1977 discovery of conducting polyacetylene. His doctoral advisor, Prof. Leroy, had worked with Raymond Daudel in Paris. At that time, zero differential overlap (ZDO) approximation was applied extensively to reduce the N^4 dependence to an N^2 dependence. Leroy's interests were mainly in supplying a theoretical background to the ZDO approximation and in proposing a more adaptable methodology for better parameterization in estimations of experimental spectral properties. The pioneering work by André and Leroy inspired quantum chemistry for periodic systems.

During his PhD studies, Jean-Marie attended the 1966 Löwdin Summer School in Sweden—an experience that strongly impacted his scientific career. The school's director, Per-Olov Löwdin (1916–2000), contributed enormously to the development of quantum chemistry and to the unity of the international quantum chemistry community. He was the founder of the Uppsala Summer School, the Gainesville Winter School, as well as the Sanibel Symposium; in addition, he contributed to the first issue of *Advances in Quantum Chemistry*, the first issue of the *International Journal of Quantum Chemistry*, the first International Congress of Quantum Chemistry, and The International Academy of Quantum Molecular Science (along with Raymond Daudel, Robert Parr, John Pople, and Bernard Pullman).

Jean-Marie's Ph.D. research spanned the borderline between solid-state physics and quantum chemistry. The periodic systems he examined are still of great interest today: an infinite 1D chain of polyene (polyacetylene) and a 2D sheet of graphite (graphene), which he exploed with both a Hückel model and a PPP semi-empirical method. These works supplied the main content of his dissertation.

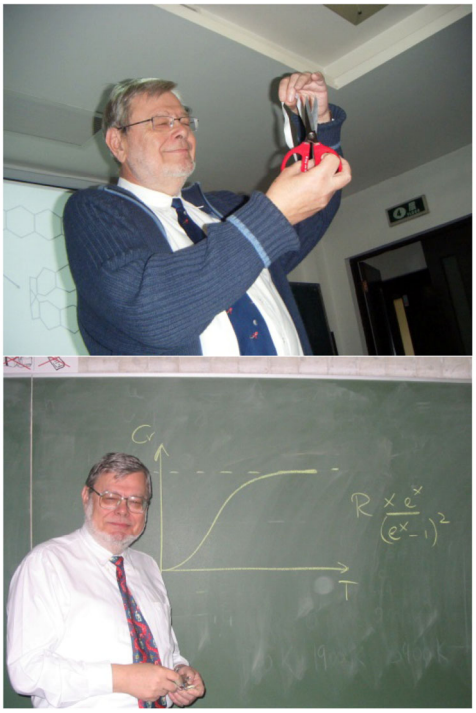
After his graduation in 1968, Jean-Marie went to IBM in San Jose to pursuit a postdoctoral research with Enrico Clementi, who pushed Jean-Marie to create a computational program for polymer band structure at the *ab initio* level. This work eventually led to the birth of the POLYMOL package. Next, Jean-Marie obtained an offer from the newly founded University of Namur (Facultés Universitaires Notre-Dame de la Paix) in Belgium to build an independent research group, which he named as Chimie Théorique Appliquée (Applied Theoretical Chemistry) and oversaw for the next 40 years. After Jean-Marie's retirement, his former student Dr. Benoît Champagne was nominated as successor at the chair of quantum chemistry in 2009, and the name of the laboratory was changed from CTA (Chimie Théorique Appliquée) to LCT (Laboratoire de Chimie Théorique). In the line of the previous CTA, the LCT continues to develop an expertise in theoretical and quantum chemistry.

It is easy to list groundbreaking contributions produced by this laboratory; they include the first quantum chemistry package for the band structure of periodic systems especially for polymers, the electronic structure of doping in polymers, the theoretical design strategy of low-band gap polymers (the last was mainly accomplished by Jean-Marie's student, the research associate Jean-Luc Brédas), and computational methodologies for both electronic and vibrational contributions to nonlinear optical responses. The University of Namur has become known worldwide for its research in chemistry and physics, to which Jean-Marie made eminent contributions.

In 1984, Jean-Marie was awarded the annual medal of the International Academy of Quantum Molecular Science (IAQMS)—an important international distinction. In 1991, he received from his Majesty King Baudouin the Francqui

Prize, the highest Belgian scientific distinction. Since 1992 he has been a member of the Royal Academy of Science, Letters and Fine Arts of Belgium and became its president in 2008. He also served as the president of the Collège Belgique from 2008 (the year it was founded) to 2011.

Presently, Jean-Marie pursues his teaching three months a year as a guest professor at Tsinghua University in Beijing. He is an honorary fellow of the Chinese Chemical Society, a Doctor Honoris Causa at the University of Warsaw, and a concurrent professor at Nanjing University. As a member of several international academies, he has given more than 250 lectures around the world. He is the author or coauthor of five books and more than 330 scientific papers.



Jean-Marie in the classroom

Jean-Marie is not only an original scientist but also an excellent teacher. He often quotes Roald Hoffmann's remark that "The desire to teach others enhanced by being obliged to teach others leads to greater creativity in research." He loves to teach as much as he loves to learn new things. In Namur, his courses included Mathematics for Chemists, Introduction to Quantum Theory, Chemical Physics, Relativistic Quantum Chemistry, and Nonequilibrium Thermodynamics.

Jean-Marie also possesses a lifelong passion for music. He started to play piano in childhood, and has collected almost all of the classical piano scores. During his stay in Beijing, he spent one whole day each week in a Xidan bookstore searching for Chinese music scores, from folk songs to piano concertos. His favorite Chinese music is *Butterfly Lover* ("Liang Zhu" in Chinese, a violin concerto) and the *Yellow River Piano Concerto* (by Yin Chengzong and Chu Wanghua, based on the *Yellow River Cantata* by Xian Xinghai). He often presents lectures about music, and is a member of the board of the Institut de Musique et de Pédagogie in Namur, Belgium.

I first met Jean-Marie in 1990 when I started my postdoc research at the University of Mons with Prof. Jean-Luc Brédas, who had just left the Namur group to build his own laboratory. So Jean-Marie is my scientific grandfather. Since becoming an emeritus in 2009, he has visited Tsinghua University for three months each year to teach graduate students about polymer electronic structure, statistics and thermodynamics, and quantum information and quantum computation.

I feel deeply honored to have organized this symposium, which turned out to be successful, and to edit this special issue to celebrate this special man. Happy birthday, Jean-Marie.

SHUAI ZhiGang (Tsinghua University)
Guest Editor

ZhiGang Shuai obtained his B.Sc. from Sun Yat-sen University (Guangzhou) in 1983 and Ph.D. from Fudan University (Shanghai) in 1989 supervised by Prof. Xin Sun. Then, he finished his postdoc research in the University of Mons, Belgium, under the direction of Prof. Jean-Luc Brédas. In 2000, he was granted the "Hundre-Talent Program" at the Institute of Chemistry of the Chinese Academy of Sciences in Beijing and became a research professor there. Since 2008, he moved to the Department of Chemistry, Tsinghua University. His research interests are theoretical chemistry and modeling of the organic functional materials for the opto-electronic properties. He has published 293 SCI paper with h-index 50. He received the National Science Fund for Distinguished Young Scholars (2004) from the National Natural Science Foundation of China, the Changjiang Scholar Professorship (2008) from the Ministry of Education, and the Chinese Chemical Society-AkzoNobel Chemical Sciences Award (2012). He is an elected Member of the International Academy of Quantum Molecular Science (2008) and the Fellow of the Royal Academy of Belgium (2013). Since 2008, he served in the editorial board of *SCIENCE CHINA Chemistry*.