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INTRODUCTION



Preface: Dieter Cremer's scientific journey

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Growing up in the Bergische Land Dieter Cremer was born in 1944 in Bad Godesberg located along the hills and cliffs of the west bank of the Rhine River, in Bonn, Germany. Because of the exacerbation of World War II, the Cremer family fled to the Bergisches Land where they found shelter on a remote farm. Dieter grew up enjoying country life and an adventurous four-hour walk through the woods to his elementary school. This experience shaped his passion and care for nature and our environment.

After the war his parents bought a house at the border of the Bergisches Land near the train station to Cologne, so that Dieter could reach the famous Albertus Magnus Gymnasium (high school) by a three-hour train ride. He was a bright student and he developed a special interest in travel and the exploration of other cultures, being inspired by the stamps he collected from his father's world-wide coffee import business correspondence. Due to his father's illness, Dieter had to leave high school, take over the coffee business during the day and attend night school. Nevertheless, he successfully finished high school with the strong support of his teachers.

From Kafka to Chemistry In 1963 Dieter enrolled as a freshman student at the Albertus Magnus University in Cologne. He began studying German language and literature, focussing on the Russian Intelligentsia and Franz Kafka. His long-term goal was to become a journalist and travel to all those countries represented in his stamp collection. Dieter needed a stipend. However, there was a lot of competition for the few stipends in the humanities, while there were more stipends available in the sciences, so he applied. He was awarded a prestigious scholarship of the *Studienstiftung des Deutschen Volkes* (German Academic Scholarship Foundation) in 1964, and as a consequence Dieter's area of study shifted to chemistry. With the scholarship and guidance from a personal mentor, he started to enjoy the sciences. After following his dream to

explore the Middle East, Pakistan and India, he then fully devoted to chemistry in 1965.

He completed his undergraduate research work in the laboratory of renowned Professor Emanuel Vogel working on the synthesis of bridged annulenes. At the end of this work, Dieter concluded that the analysis of these compounds via NMR spectroscopy was more interesting and attractive than the time-consuming multi-step synthesis. Therefore, he joined Professor Harald Günther, the NMR specialist in the chemistry department. Dieter successfully finished his diploma work on NMR spectroscopy of unsaturated compounds with summa cum laude. Before proceeding to his doctoral work, he attended Professor Per-Olov Löwdin's famous quantum chemistry summer school in Uppsala, Sweden. This turned into a pivotal point in Dieter's career. After the summer school he concluded that analysis by calculation was even more attractive than analysis by measurement. Professor Günther was very supportive and gave Dieter a theoretical thesis topic, *Semiempirical MO studies on Cyclic Hydrocarbons*, which Dieter mastered in two years, again with summa cum laude. After his Ph.D. he followed Professor Günther's recommendation to join Nobel Laureate Professor John Pople at Carnegie-Mellon University in order to learn more about the theory of NMR spectroscopy.

Postdoctoral years with Nobel Laureate John Pople However, when Dieter arrived in the fall of 1972 at Carnegie Mellon equipped with a scholarship of the German Science Foundation, Professor Pople had already moved to *ab initio* theory and the GAUSSIAN program. Dieter took the chance and engaged in this hot topic, acquired excellent programming and method development skills and as a result, his work with Professor Pople culminated in a number of high-ranking publications including the landmark paper on the Cremer-Pople puckering coordinates.

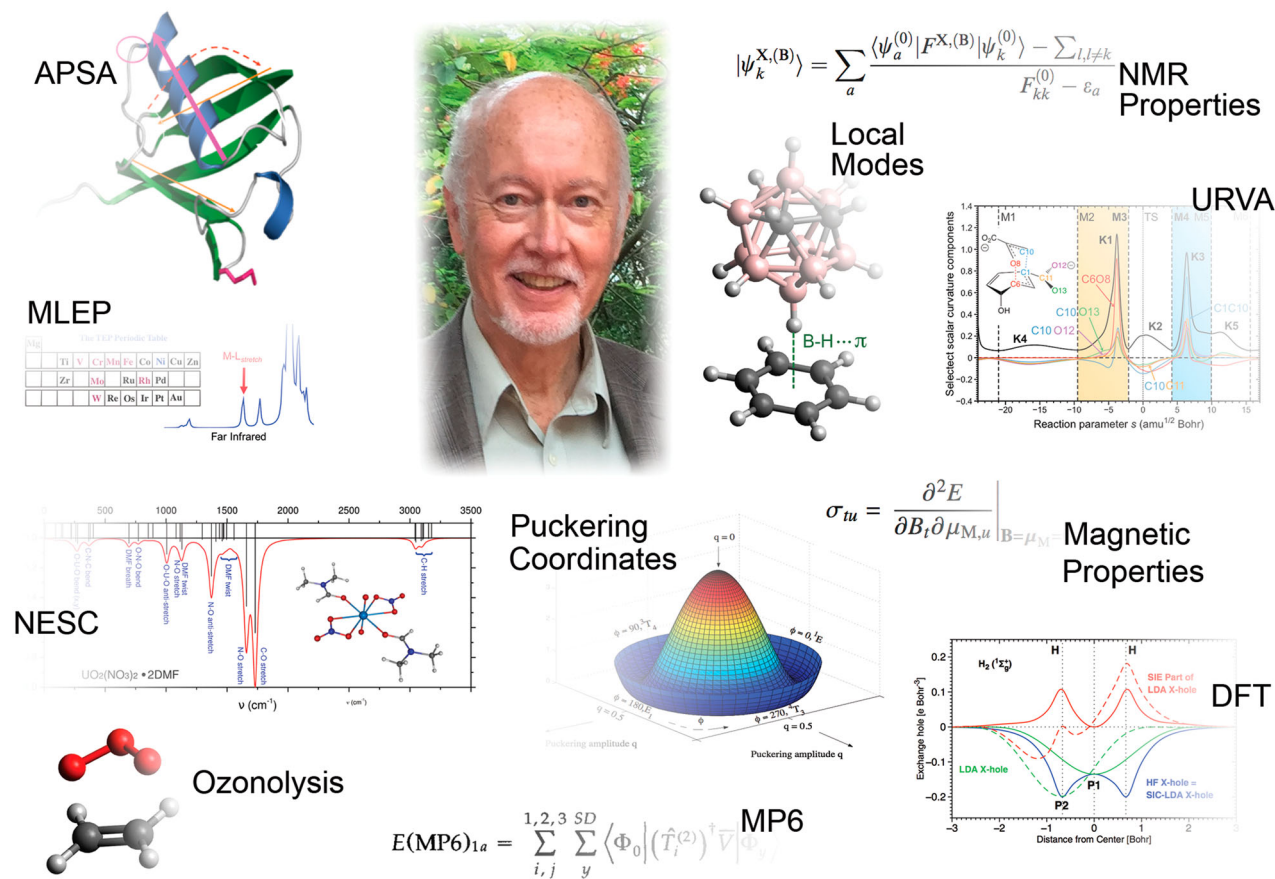


Figure 1. Some Highlights of Dieter Cremer's (1944–2017) Contributions to Theoretical Chemistry.

In 1974, Dieter returned to the University of Cologne starting his own academic career, very well prepared and equipped with the unique combination of knowledge in organic chemistry and spectroscopy; knowledge of quantum chemistry and physics; programming and mathematical skills, as well as professional writing skills. This led to the outstanding breadth and diversity of Dieter's research, some of which will be highlighted in the following (Figure 1).

University of Cologne (1975–1990) It all began in 1975 with Dieter's extensive *ab initio* studies on ozonolysis reactions, verifying the three-step mechanism of the ozonolysis of alkenes suggested by Criegee. He could identify the formation of OH radicals in the gas phase ozonolysis of alkyl substituted alkenes as the most likely process, which has important consequences for the chemistry of our atmosphere.

In 1980 Dieter met Professor Richard Bader and learned about his fascinating Quantum Theory of Atoms in Molecules (QTAIM). Dieter was the first who made QTAIM understandable for the average chemists and applied Bader's theory to solve real life problems. For this seminal work he received the Academy of Science

Award in Chemistry in 1984 as one of the first theoretical chemists. One often cited example is Dieter prediction of helium compounds in 1987, first strongly criticised but proved and accepted approximately 16 years later. Another highlight from this time is Dieter's work on analytical derivatives for post-SCF methods, which are essential for the calculation of response properties.

Gothenburg University (1990–2005) In 1990 Dieter accepted an offer at the University of Gothenburg in Sweden to establish a new Institute of Theoretical Chemistry. He served as academic director of this institute until 2005. He established a systematic and in-depth education and training in theoretical and computational chemistry at the undergraduate and graduate level. He also served as chairman of the Scandinavian HPC committee in Linköping, Sweden's first national supercomputer centre. Some highlights from this time include the development, coding and testing of the first Møller Plesset 6th order program, which turned out to be a unique tool for the analysis and classification of post-SCF methods, in particular to predict full CI energies and to study the convergence behaviour of the MP series. He also developed a program package for the calculation of magnetic

properties including NMR chemical shifts and NMR spin-spin coupling constants. Another important project he started in Sweden was the systematic development of relativistic DFT and relativistic wave-function methods.

Besides magnetic properties, Dieter started to think about how one could use all the information embedded in an IR or Raman spectrum in the best possible way. His major target was to develop a bond strength measure based on vibrational spectroscopy. This led to his famous idea of local vibration modes being based on mass-decoupled Euler-Lagrange equations. The local vibrational modes turned out to be one of the essential features of the Unified Reaction Valley Approach (URVA), which characterises each step of a chemical reaction in terms of the curvature of the reaction path that the reacting compounds trace on the potential energy surface.

The University of the Pacific (2005–2009) In 2005 Dieter joined the University of the Pacific, Stockton, CA as Professor of Chemistry and Professor of Physics to establish a strong Theoretical Chemistry Research unit. The Provost asked him to think about a new nanotechnology class for science students, an emerging field at that time. Although this was new territory for Dieter, he created and developed the curriculum for a one of a kind new four-year nanotechnology major, including 12 new nanotechnology core courses. This is a typical example for Dieter's curiosity for life-long learning and exploring new things. Whatever he did, he did it 100% perfect.

A major research highlight during this time was the development of the *Automated Protein Structure Analysis* (ASPA), representing the protein backbone as a smooth line in three-dimensional space, which can be accurately described by its curvature and torsions.

Southern Methodist University (2009–2017) In 2009 Dieter joined SMU as Professor of Chemistry and Director of the Computational and Theoretical Chemistry Group (CATCO). Major objectives included the installation of a strong computational and theoretical chemistry research program, bringing high performance computing to the campus, and to engage in the development of a new Ph.D. program in Theoretical and Computational Chemistry, which has all been accomplished by now.

At SMU Dieter excelled his relativistic programs to the next level by adding higher derivatives, new response properties, and spin-orbit coupling. He could deliver the important proof that his local vibrational modes are uniquely connected to the vibrational normal modes, and that the related local mode force constants are a unique measure of the intrinsic bond strength for covalent bonds as well as weak interactions including hydrogen, halogen, pnictogen, chalcogen and tetrel bonding. In collaboration with Nanjing University, he could identify a new type

of B-H... π bond, and he realised a new understanding of hydrogen bonding in water clusters explaining for the first time at the atomic level why warm water freezes faster than cold water. He stepped up URVA to allow the analysis of reactions in both, gas phase, solution or even in an enzyme. More than 600 catalysis reactions were analysed, and the results were unified in a reaction library.

Dieter Cremer and the Austin Symposium on Molecular Structure and Dynamics (ASMD) For the last 50 years the ASMDs have been important gathering points for experts in diffraction methods, spectroscopy, and computational chemistry to present and discuss novel methods and techniques, unusual molecular structures, and interesting reaction dynamics. ASMDs have been often the incubator of new research projects and in more than one case initialised work that was recognised by the Nobel committee.

The Austin Symposium started in 1960 under the name *Gasphase Molecular Structure Meeting* to bring crystallographers and microwave spectroscopists together. It developed into a biannual meeting organised by Professor James E. Boggs in Austin. In 1980, the words *Gas Phase* were dropped, the name *Austin Symposium on Molecular Structure and Dynamics* was coined, and the first theoreticians were invited. One of them was Dieter who attended 5 additional ASMD meetings in the following years.

In 2012, the ASMD moved to Dallas, became the ASMD at Dallas (ASMD@D), and the 24th Symposium was organised for the first time by CATCO at Southern Methodist University, Dallas, Texas, USA. CATCO organised the 25th Austin Symposium, March 2014 in memoriam of James E. Boggs and also organised the 26th Symposium, March 2016 celebrating 50 years of ASMDs.

The 27th Annual Symposium in 2018 was dedicated in memoriam of Dieter Cremer (1944–2017), who served as Chairman of the 2012, 2014, and 2016 ASMD@D meetings vitalising the symposia with many new refreshing ideas and inspiring scientific discussions. More than 100 participants from 22 countries contributed to the success of this special symposium. At the end of the conference it was decided to honour Dieter Cremer's scientific achievements with a special volume of *Molecular Physics* inviting the conference attendees to contribute as well as Dieter's colleagues who could not attend the meeting, which led to this impressive issue.

Dieter Cremer's legacy Dieter was an exceptionally gifted teacher and lecturer. He presented each lecture or talk as an exciting story well-seasoned with little anecdotes attracting the attention of his audience benefitting from his humanistic studies. He was also a

dedicated mentor preparing each student in the best possible way for his/her future carrier. He supervised nearly 90 graduate students, 20 postdoctoral associates, and over 40 undergraduates. 19 of the graduate and postgraduate students he supervised have since become professors at universities in seven different countries around the world.

Dieter's knowledge always served him as an inexhaustible source of new ideas, which made CATCO to what it is now, an incubator for the development of new methods and their application to pending chemical problems. Dieter's legacy will live on in CATCO and all members are devoted to continuing in his spirit. We hope that this memorial issue serves as an inspiration for all colleagues in the field of theoretical chemistry and beyond, in particular for young and upcoming scientists to proceed in their own work with the care, dedication, and inspiration that Dieter expounded.

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Disclosure statement

No potential conflict of interest was reported by the author.