

## Jörg Fleischhauer 75

*This Special Issue of 'Zeitschrift für Naturforschung, Series A' is dedicated to Professor Jörg Fleischhauer on the occasion of his 75th birthday in recognition of his achievements as a scientist and as an academic teacher.*

Jörg Fleischhauer was born on August 22, 1939 in Dresden (Saxony). After attending elementary school from 1946 till 1951 in Eisenach (Thuringia), he moved with his family to Hagen (Westphalia) and received his qualification for university entrance (Abitur, i.e. A-levels) in 1959.

In the summer semester of 1959, he started to study chemistry and physics at the Rheinische Friedrich-Wilhelms-Universität in Bonn. He passed his final chemistry examination successfully on February 18, 1966 obtaining his diploma. The chemisorption of metal atoms on metal surfaces was the topic of his diploma thesis which he wrote under the supervision of Prof. Dr. H. Moesta (Bonn) from March till November 1966. He passed his final examination in physics successfully on July 28, 1968. Being under the supervision of Prof. Dr. F. Korte, he started working on his doctoral thesis entitled 'Quantenmechanische Rechnungen zur Deutung von Kettenlängeneffekten bei der Nitrierung von Methylalkyldihydrochinon-äthern (Quantum-Chemical Calculations on the Interpretation of the Effect of the Chain Length in the Nitration of Methylalkyldihydrochinon Ethers)' in February 1967. Finishing this work in October 1968, he received his Dr. rer. nat. degree. During this time, he was also supported by Priv.-Doz. Dr. H. D. Scharf, which led to a long-lasting cooperation.

After receiving his doctoral degree, he spent the time from 1969 till 1974 as a scientific assistant in Prof. Dr. H. D. Scharf's research group working on his habilitation thesis in the field of theoretical organic chemistry. Upon finishing his thesis entitled 'Betrachtung von Struktur- und Reaktionsparametern mit LCAO-MO-Theorien (Study of Structure and Reactivity Parameters with LCAO-MO Theories)', he was appointed professor in the field of theoretical chemistry at the Rheinisch-Westfälischen Technischen Hochschule



Aachen (RWTH) in 1974. Accepting the call, he established this field of research at the RWTH and represented it in research and teaching for a period of 30 years. Even before his habilitation, he performed pioneering work in the field of the calculation of circular dichroism (CD) spectra in 1972 when he studied in the atypically negative Soret band of an insect haemoglobin with the simplest computational means in close cooperation with his experimentally working colleague Axel Wollmer. With this work he, laid the foundations for the quantum-chemical study of the circular dichroism of proteins and peptides in Germany. In the following years, he developed computer programs which, based on the perturbation theory of Tinoco and the matrix method of Bayley and Schelman derived thereof, allowed computer-assisted calculations of the CD of peptides, proteins, and nucleic acids. These programs were not only used in cooperation with research groups at home and abroad, but were also given, upon request, free of charge to research groups all over the world. Even ten years after Jörg Fleischhauer's retire-

ment the demand for these program codes is still continuing. Another code developed by Jörg Fleischhauer and his group on the basis of a modified semiempirical program permits the calculation of monopoles used in the matrix elements of the perturbation operator in the program to calculate the CD of biomacromolecules. A close cooperation in the field of the CD of peptides and proteins with Robert Woody still persists.

In addition to this software, Jörg Fleischhauer and his group developed a program code which based on available semiempirical configuration interaction (CI) programs made possible the calculation of the circular dichroism of small molecules and, therefore, allowed the determination of the absolute configuration of such molecules which could not be subjected to X-ray structure determination. These programs were given to research groups upon request as well. Most of the later work of Jörg Fleischhauer and his coworkers on small molecules was performed by employing the time-dependent density functional theory and commercially available programs. Besides his work in the field of CD spectroscopy, Jörg Fleischhauer also investigates the theoretical aspects of the magnetic circular dichroism (MCD), working in close cooperation with Josef Michl.

Jörg Fleischhauer published more than 100 scientific papers and book chapters on different fields of theoretical chemistry and spectroscopy. 18 students received a doctor's degree under his supervision, five of which became professors. Besides lectures and seminars, Jörg Fleischhauer could always be approached by students to explain the sometimes complicated aspects of theoretical chemistry.

In the name of his former students and coworkers and also in the name of the editor and the editorial office of this journal, we wish Jörg Fleischhauer many more years of health and contentedness.

Gerhard Raabe  
Aachen

Gernot Frenking  
Marburg

*Gerhard Raabe:* Born in 1950. After his training as a chemical laboratory technician (Farbenfabriken Bayer AG, Leverkusen 1967–1970), military service (1970–1972) and 'Abitur' (1974), he started studying chemistry in the summer semester of 1975 at

the RWTH Aachen. He received his diploma in 1980 (J. Fleischhauer) and his Dr. rer. nat degree in 1984 (J. Fleischhauer). From 1984 till 1985, he worked as a postdoc in the research group of J. Michl (University of Utah, Salt Lake City). Starting in 1987, he worked as a 'Product Development Manager' with AKZO Chemicals in Düren (Germany) till 1988. Since 1989 he was a scientific assistant in the department of Organic Chemistry of the RWTH Aachen. His habilitation in the field of theoretical chemistry took place in 1998. Gerhard Raabe was appointed associate professor in 2003 (RWTH Aachen). His working fields are quantum chemistry, CD spectroscopy, and X-ray structure determination. Fellowships: 'Promotionsstipendium' by the 'Studienstiftung des deutschen Volkes' 1981–1983, 'Special Fellowship Award by the 'Studienstiftung des Deutschen Volkes' 1984–1985.

*Gernot Frenking:* Born 1946. After apprenticeship as chemical laboratory technician (Farbenfabriken Bayer AG, Uerdingen 1961–1964) and further employment (1964–1966) followed by 'Abitur' (1969), he started studying chemistry in the winter semester 1969/70 at the RWTH Aachen where he received his diploma in 1973 (H. D. Scharf and J. Fleischhauer). He was a research student for two years with Kenichi Fujii at Kyoto University (1974–1976) before he carried out his doctoral work at the TU Berlin (1976–1979, H. Götz). This was followed by his habilitation in Theoretical Organic Chemistry at the TU Berlin (1979–1984). After a research stay at the University of California, Berkeley (1984–1985) and employment as staff scientist at the Stanford Research Institute, Menlo Park (1985–1989), he was appointed C3 (Associated) professor for Computational Chemistry at Philipps-University Marburg (1990) where he became C4 (Full) professor in 1998. His research interests are molecular quantum chemistry, analysis of chemical bonding, molecules with unusual bonds, and theoretical studies of reaction mechanisms. Awards: Elhuyar-Goldschmidt Prize of the Royal Society of Chemistry of Spain (2007), Fellow of the Royal Society of Chemistry (FRSC, 2008), Schrödinger Medal of the WATOC (2009), The Hofman Distinguished Lecture, Imperial College, London (2010), The Lise-Meitner Lecturer, The Hebrew University of Jerusalem, Israel (2011), Hans-Hellmann-Professor at the Philipps-University Marburg (2012).