Theor Chem Acc (2005) 114: 253–254
DOI 10.1007/s00214-005-0694-4

EDITORIAL

Michael Dolg · Peter Botschwina

Hermann Stoll

Published online: 26 September 2005

This issue of *Theoretical Chemistry Accounts* is dedicated to Professor Hermann Stoll on the occasion of his sixtieth birthday. Hermann Stoll was born on October 28th, 1945 in Bissingen/Teck. After his military duty he started to study physics in October 1966 at the Technische Hochschule (later University) of Stuttgart, being supported by the Studienstiftung des Deutschen Volkes. In early 1971 he joined the Institute of Theoretical Chemistry (at that time housed in a beautiful villa in Relenbergstraße in the upper area of Stuttgart) which had been established only a couple of years earlier at the University of Stuttgart under the directorship of Heinzwerner Preuß and was one of the first centers for quantum chemistry in Germany. At that time several scientists now holding professor positions in Germany or Austria worked in the group, e.g., Karl Jug was a long-term visiting professor, Wilfried Meyer and Rudolf Janoschek were scientific assistants and Peter Botschwina was a research student. Hermann carried out a diploma thesis entitled "SCF-Berechnung von Elektronenzuständen in kleinen Atomaggregaten im Zwischenbereich zwischen Einzelatom und Festkörper" which may be classified as pioneering ab initio work in theoretical cluster physics, well before this field became a part of main-stream research. He received the degree of a "Diplomphysiker" in early 1972 and took over Wilfried Meyer's position in August 1973. Within the remarkably short time of only two years, Hermann managed to complete almost independently a both ambitious and successful doctoral thesis entitled "Hartree-Fock-Berechnung von Kristallenergien und Gleichgewichtsstrukturen für Lithium, Beryllium und Lithiumhydrid". Several ideas and equations from this work were used by him and his coworkers about 25 years later to perform in the basis of Wannier-type orbitals the first correlated ab initio study of a three-dimensional periodic system, i.e., a full CI study of crystalline lithium hydride. In 1978 Hermann completed his habilitation thesis entitled "Die direkte Berechnung von lokalisierten Orbitalen und lokalen Korrelationskorrekturen in Molekülen und Festkörpern". Among many other ideas, this work contains what is known today as the Stoll-Pavlidou-Preuss (SPP) self-interaction correction in density functional theory, a simple but very efficient correction of the local density approximation (LDA) improving drastically its accuracy for systems with unpaired electrons.

After his habilitation Hermann Stoll encountered the serious problem that the number of professor positions he could apply for was very small, since most of the positions created in Germany in the early 1970s had already been occupied by scientists who were just a few years older than him. Whereas the shortage of professor positions certainly was an unpleasant situation for him, it turned out to be very beneficial for the Stuttgart Institute of Theoretical Chemistry. Hermann kept staying at this location and devoted his scientific life to keep the institute an active center of research producing excellent work in various fields of quantum chemistry and solid state physics. Scientifically he soon became a leading figure in the institute. After four years as C2 professor (1981–85) he finally got a permanent position as Akademischer Rat (1985) and Oberrat (1994). He was appointed Außerplanmäßiger Professor in February 1986. When Hans-Joachim Werner took over the directorship in 1994, Hermann continued to be the vice-director of the institute.

Starting with his habilitation work Hermann's interest in density functional theory continued over his whole scientific career. Long before modern gradient-corrected density functionals became available and popular, he and his coworkers used SPP-corrected LDA in connection with pseudopotentials to study larger systems, e.g., gas-phase clusters of alkaline and coinage metals or the adsorption of hydrogen and small metal clusters on surfaces. After Andreas Savin had joined the institute in 1981 for his doctoral thesis and subsequent habilitation Hermann also started to couple density functional approaches for the description of short-range dynamical correlation with wavefunction-based

M. Dolg (✉)
Institut für Theoretische Chemie, Universität zu Köln,
Greinstr. 4, 50939 Köln, Germany
E-mail: m.dolg@uni-koeln.de

P. Botschwina
Institut für Physikalische Chemie, Universität Göttingen,
Tammannstr. 6, 37077 Göttingen, Germany

multi-configurational ab initio treatments for long-range non-dynamical correlation effects, a topic which he still pursues in his current projects.

In the course of a long-standing cooperation with Peter Fulde and coworkers Hermann developed in the early 1990s a simple but very successful method to extend quantum chemical ab initio correlation treatments to periodic systems. The so-called incremental expansion of the correlation energy based on groups of localized orbitals in extended systems appears to be up to now the only scheme to allow the application of accurate correlation treatments such as the coupled-cluster ansatz to crystalline solids. Numerous studies providing reliable ab initio estimates of cohesive energies for simple crystals and polymers followed his pioneering work on diamond, graphite and silicon. In the meantime the incremental scheme also has been applied to evaluate ab initio correlation corrections for band structures. Possible extensions of the method to metals are currently being investigated.

Besides methodological contributions to density functional theory and local ab initio correlation schemes Hermann became interested in the use of pseudopotentials as a tool to save computer time and, a few years later, to incorporate the major relativistic effects into formally nonrelativistic quantum chemical calculations. Important contributions in the field of energy-adjusted (energy-consistent) pseudopotentials, corresponding core-polarization potentials and core-core/nucleus repulsion corrections made in the Stuttgart group since the early 1980s have been inspired or initiated by him. New parametrizations based on multi-configurational Dirac-Hartree-Fock all-electron reference calculations employing the Dirac-Coulomb-Breit Hamiltonian are currently being derived in collaborations between his group and the ones of Michael Dolg and Peter Schwerdtfeger. Without his ideas and guidance the so-called "Stuttgart pseudopotentials" would not have developed as well as they did.

The development and application of relativistic pseudopotentials led Hermann to become interested in relativistic effects in heavy and superheavy elements. Together with Evert Jan Baerends he became chairman of the first Euro-Conference on "Relativistic Effects in Chemistry and Physics" (De Haan, 1993), which marked the beginning of a very successful series of conferences.

From 1994 on, after the directorship of the institute had gone over to Hans-Joachim Werner, one of the two main authors of the MOLPRO package, Hermann found a new solid framework for many of his own developments and eventually became one of the coauthors of the program system. New world-wide cooperations could be established resulting in many publications too numerous to be dealt with here.

The scientific work of Hermann Stoll is documented in more than 230 original publications and book contributions. His 1989 work on the evaluation of correlation energies with density functionals of Becke and Lee, Yang and Parr was cited by far more than 1.000 times, and his work on relativistic pseudopotentials for the 4d- and 5d-transition metals is about to reach this number. Owing to his ongoing scientific activity in various projects and collaborations many more interesting publications are expected to come in the next years.

Despite working throughout all his career at Stuttgart University he inspired a large number of students, several of which became university teachers in theoretical chemistry or theoretical inorganic chemistry. Among these are Patricio Fuentealba, Peter Schwerdtfeger, Andreas Savin, Michael Dolg, Winfried Plass, Martin Kaupp and Thierry Leininger.

Over several decades Hermann Stoll was teaching mathematics for chemists. The classes, although not liked too much by many of the students because of the difficult subject, involved the best organized and understandable lectures one could attend in the Stuttgart chemistry department. Over the years this one-year course became such a standard routine for Hermann, that he hardly needed his lecture notes. At one particular day he even mentioned that he was too tired to follow his own lecture. Substituting him in the lectures required careful preparation, since in one or the other chapter of his manuscript a hole, created most likely by drops of sulphuric acid left on the desk in the chemistry lecture hall, had caused important formulas to be missing and thus had to be filled by the mathematical knowledge of the lecturer. Hermann's lectures on special topics of theoretical chemistry, e.g., pseudopotentials, were always very beneficial for the members of the institute.

Colleagues and students in the Stuttgart quantum chemistry group learnt to know Hermann Stoll as a very knowledgeable but modest and patient person, who was always willing to help and give his valuable advice, if he was asked for it. Whenever he was not able to answer difficult questions immediately, he used to copy them down on a sheet of paper and put them on his well-organized desk. After some time he always came up with a solution, which often looked surprisingly simple and made the questioner doubt why he was asking the question at all. The atmosphere Hermann created at the Institute of Theoretical Chemistry was scientifically professional, but personally warm and friendly. Being under his supervision as a student one often experienced a positive type of stress. After having received new advice or directions from him in the late afternoon, the next morning one would already be asked "Was gibt's Neues?" Institute members not only paid respect to him as a scientist, but also admired the length of the yearly institute excursions based on his suggestions as well as the high temperature in his office and the fact, that he still continued to wear a pullover even on the hottest days of summer.

We all, colleagues, coworkers and students, wish Hermann Stoll many more years of exciting scientific experience, and him, his wife Christiane as well as his three children all the best for the future.