Theor Chem Acc (2010) 127:109–119
DOI 10.1007/s00214-010-0812-9

Editorial

Published online: 25 September 2010

This special issue of *Theoretical Chemistry Accounts* contains a collection of papers dedicated to the memory of Jürgen Hinze, former Professor of Theoretical Chemistry at the University of Bielefeld, Germany. He was an esteemed colleague and a valued friend of many of the contributors of this issue.

We cordially thank all authors for their contributions, and we are grateful to the reviewers for their help, their constructive criticism, and their comments. We are very thankful to Robert Hinze, Edzard Klapp, Sigrid Peyerimhoff, Wolfgang W. Schoeller, and Ersin Yurtsever for biographical details. These have been included in the scientific biography of Jürgen Hinze that sketches the principal lines of his scientific work.

Last but not least, we wish to acknowledge gratefully Chris Cramer, Editor-in-chief, for giving us the opportunity to edit this issue, for his assistance, and for his patience.

Alexander Alijah (Reims, France)
Dirk Andrae (Berlin, Germany)

Theory in Chemistry, Theory for Chemistry
A scientific biography of Jürgen Hinze (1937–2008)

Portrait taken from D. Bergmann and J. Hinze, Electronegativity and Molecular Properties, Angew. Chem. Int. Ed. 35 (1996) 151. © Wiley-VCH Verlag GmbH & Co. KGaA. Reproduced with permission

Jürgen Andreas Michael Hinze was born in Berlin on June 28, 1937. His family later moved to Stuttgart, a town in the south-west of Germany, where he was brought up and completed school education, in 1957, with receipt of the general qualification for university entrance (*Abitur*). His interest in science and technology showed up early. For example, he developed very good skills in constructing model glider airplanes during his years at school, at a time when prefabricated or even ready-to-fly assembly kits were unavailable. Many years later, he could still enthusiastically tell about problems related to wing profiles, but also remembered his teachers' regretful comments that his marks in the languages were not as good as those in mathematics and the sciences.

In 1957, Jürgen began studying chemistry at the *Technische Hochschule Stuttgart* (renamed to *Universität Stuttgart* ten years later). After completion of the first part of the studies (*Vordiplom*) in 1959, he moved to the U.S.A. in 1960. A Fulbright scholarship allowed him to go to the University of Cincinnati, Ohio, where he wrote his thesis on electronegativity under the guidance of Hans H. Jaffé (1919–1989). The new concept of orbital electronegativity was developed in this work, and the resulting new electronegativity scale, widely known in chemistry textbooks by the name Mulliken-Jaffé scale, provides electronegativity values depending on the valence state an atom assumes in a molecule. In this way, e.g., a carbon atom is assigned a higher electronegativity in an ethynyl group (sp hybridization) than in a methyl group (sp^3 hybridization), so that needs of experience could be met.

From 1962 to 1964, Jürgen was postdoctoral fellow with Kenneth S. Pitzer (1914–1997) at the Rice University in Houston, Texas. His research subjects during that stay were not restricted to Theoretical Chemistry. In addition to the question of bonding in noble gas halides and the calculation of atomic integrals with integrands containing factors depending on interelectronic distances, he also joined Robert F. Curl, Jr. (*1933), in the study of the molecule CH_2=N–CH_3, the simplest Schiff base. Jürgen prepared this highly thermolabile substance by pyrolysis of an *s*-triazine precursor, recorded, and analyzed its infrared spectrum in the solid and in an argon matrix and was also involved in the analysis of its microwave and ^{1}H NMR spectra.

Thereafter, he worked as an assistant at the Institute of Physical Chemistry of the *Technische Hochschule Stuttgart*, with Theodor Förster (1910–1974), but soon left Germany again, in 1966, and went to the Laboratory for Molecular Structure and Spectra (LMSS) at the University of Chicago, Illinois. The LMSS, chaired at that time by Robert S. Mulliken (1896–1986) and Clemens C. J. Roothaan (*1918), was one of the 'hot spots' of method development in electronic structure theory. In that same year, Mulliken was awarded the Nobel Prize in Chemistry. Jürgen joined Roothaan's group and developed computer programs for multiconfiguration self-consistent field (MCSCF) calculations, first for atoms and then for diatomic molecules. To younger people, complaining about difficulties of program development, he sometimes told the story about writing his first computer programs. Initially, following Roothaan's notes, as copied from a blackboard, he had to use machine-dependent assembler language and faced severe storage limitations (compared to present-day standards). High-level programming languages were not yet available, and the principles of object-oriented programming still widely unknown.

Just about one year after having entered the LMSS, Jürgen became Assistant Professor at the Department of Chemistry of the University of Chicago. He stayed there till 1975, with a short interruption by half a year's sabbatical spent in 1973 at the *Max-Planck-Institut für Physik und Astrophysik* at Munich. Around 1970, he switched the spelling of his first name from 'Jürgen' to 'Juergen' when indicating his authorship on a publication. His major research subject during these years was the development of the MCSCF method for electronic structure calculations. With his first doctoral student, Bowen Liu, he engaged in the development of an MCSCF program for larger linear molecules (with more than two nuclei), a joint research project with Enrico Clementi's group from the IBM Research Laboratories at San Jose, California. As in all previous work, Slater-type functions were to be used in this project too. Bowen decided to move to San Jose for the main work of code development, so that Juergen became co-supervisor, together with Doug McLean, of Bowen's

thesis on theoretical studies of the three-electron systems He_2^+ and linear H_3 [1, 2]. The already existing MCSCF code for diatomic molecules was applied and developed further in three other research projects. Kate Kirby (Docken), now retired Director of the Institute for Theoretical Atomic, Molecular and Optical Physics (ITAMP) at the Harvard-Smithsonian Center for Astrophysics, Cambridge, Massachusetts, studied spectroscopic properties of low-lying singlet and triplet states of lithium hydride. A study of the five lowest electronic states of carbon hydride, a species of astrophysical interest, was carried out by George Lie. The first paper published from his work was included later in an 'incomplete list of landmark papers in ab initio molecular electronic structure methods' [3]. Furthermore, his work provided the basis for the prediction of the lambda-doubling spectrum of ^{13}CH by Don Levy and Juergen in 1977. The high quality of their prediction was confirmed about ten years later by an analysis of new experimental data [4]. The valence excited states of sodium hydride were studied by Edward Sachs. His work finally helped to understand the broadening of the sodium *D* line induced by collisions between sodium and hydrogen atoms. In addition, a semiempirical version of the MCSCF method was developed, with Charles Eaker, and used to investigate possible reaction paths in the thermal decomposition of 1,2-dioxetane. The general work on the development of the MCSCF method clearly showed the limitations caused by the use of algebraic basis sets. This observation led Juergen to initiate a feasibility study for a fully numerical Hartree-Fock method for molecules, which became the topic of Frank Tobin's thesis.

In 1975, Juergen was appointed Full Professor at the *Universität Bielefeld* (founded in 1969) and thus became one of the four founding professors of the chemistry department. Juergen stayed at Bielefeld until his retirement in 2002. The move from the excellent University of Chicago to Bielefeld was not easy for him; however, he liked the challenge to build up something new in his native country, Germany. The Bielefeld Center for Interdisciplinary Research (*Zentrum für interdisziplinäre Forschung*, ZiF), an internationally operating Institute for Advanced Study founded already in 1968, played a crucial role in the following years. It provided, and still provides, excellent facilities as a conference center and for hosting groups of researches for longer periods of time up to a year. Juergen initiated and organized research groups at the ZiF in the years 1978–1980 and 1996–1997. The international conferences, related with these activities, united chemists, physicists, and mathematicians around interdisciplinary topics and attracted much attention across the disciplines. The proceedings of seven workshops, held in the first period of time mentioned above, were edited by Juergen and published in the form of five books. The lists of contributing authors read like a 'who's who' in contemporary research in the fields of atomic, molecular and optical physics, theoretical chemistry, and in several branches of mathematics.

Juergen always tried to push theoretical work to the point where calculated results could be compared directly with observed quantities. With Lüder Engelbrecht, a postdoc coming from Dieter Sutter's group at the *Universität Kiel*, Germany, he presented in the late 1970s a rigorous and a very detailed analysis of the requirements that have to be met to actually reach coincidence between theoretical and experimental results for spectroscopic properties of small molecules.

Also in the late 1970s, the development of sophisticated methods for the treatment of electron correlation in electronic structure theory continued to be one of Juergen's principal research subjects. Together with Alojzy Gołębiewski from the Jagiellonian University at Cracow, Poland, and Ersin Yurtsever, who came as a postdoc from Donald Shillady's group at Virginia Commonwealth University, Richmond, Virginia, new algorithms for solving the general MCSCF problem in its algebraic version were developed and implemented. Ersin Yurtsever is now Professor and Dean of the Faculty of Arts and Sciences at Koç University, Istanbul, Turkey. Reduced density matrix elements for general reference state functions were considered already around 1980 as basic quantities to evaluate configuration interaction (CI) energies in joint work with John Broad. He came as a postdoc from Bill Reinhardt's group, which was at that time at the University of Colorado, Boulder, Colorado. With the computer scientist K. V. Dinesha, now Professor at the International Institute of Information Technology at Bangalore, India, the merits of permutation group algebra in evaluating CI matrix elements for atoms were explored.

The fully numerical, i.e., basis-set-free, approach to the atomic or molecular (MC)SCF problem was also pursued further. Initially, the molecular problem was treated in terms of one-center expansions for the orbitals. Thomas Vögel, Juergen's first doctoral student at Bielefeld, considered multicenter expansions for the orbitals and applied the numerical SCF method to H_2^+ and H_2; he completed his thesis in 1981. The mathematician Friedrich Biegler-König joined Juergen's group in the mid 1980s. He returned to Bielefeld from a postdoc stay with Richard F. W. Bader at the Department of Chemistry, McMaster University, Hamilton, Ontario, Canada, where he had contributed to the development of mathematical methods required for the topological electron density analysis (wherefrom evolved what is known today as the Quantum Theory of Atoms in Molecules, QTAIM). With Juergen he developed and implemented new efficient algorithms for numerical atomic MCSCF calculations. Friedrich

Biegler-König is now Professor at the *Fachhochschule Bielefeld*, an advanced technical college. External (electric or magnetic) fields were also included in the numerical approach, as shown in the work of Alexander Alijah, who completed his thesis on the photodissociation of the hydrogen atom in strong magnetic fields in 1988. The 1990s then saw several interesting developments conducted under Juergen's supervision: the creation of a two-dimensional numerical SCF program for relativistic four-component electronic structure calculations for closed-shell states of diatomic molecules by Hans-Dieter Krumme (1992); further work on the numerical MCSCF problem for atoms, with extension to the case including an external static electric field, by Johannes Stiehler (1995); the development of programs for time-dependent numerical MCSCF and CI calculations on atoms by Martina Rosenberger (1997); and the generation of a program for relativistic four-component numerical MCSCF calculations on atoms by Markus Reiher (1998). Markus Reiher is now Professor at the Swiss Federal Institute of Technology at Zurich, Switzerland. With Dirk Andrae, who came as a postdoc from the group of Heinzwerner Preuß and Hermann Stoll at the *Universität Stuttgart*, a numerical Kohn–Sham program for closed-shell atomic states was set up. It included several exchange- and correlation-energy density functionals, based on the local density and the generalized gradient approximations, with explicit construction of the functional derivatives in the SCF procedure. From the many papers resulting from these developments, the one written together with Johannes Stiehler on static electric dipole polarizabilities and hyperpolarizabilities for all atoms from He to Kr stands out for the large amount of accurate data, for the wide range of systems considered, many of them being open-shell cases and excited states, and for the many references included that make it an "excellent source for theoretical data" [5].

The concept of electronegativity, which Juergen had generalized to an orbital-dependent quantity in his thesis, starting from Mulliken's definition, was revisited in the early 1980s. The orbital electronegativity was extended such that it became dependent not only on hybridization, but also on partial atomic charge. This opened the way to the definition of orbital electronegativities of molecular fragments or group electronegativities. Juergen showed, together with Dieter Bergmann, that group electronegativities and partial charges, computed for a large number of molecules, correlate well with several experimentally accessible quantities (bond lengths and bond dissociation energies, NMR and ESCA chemical shifts, proton affinities, force constants). Simple, but remarkably reliable models were obtained for the prediction of these molecular properties.

Another area of Juergen's research deserves mention: the development of accurate methods for the theoretical study of collision and scattering processes and for quantum dynamics in small molecules. The ZiF research group activities in the late 1970s and his getting to know John Broad may be seen as events triggering Juergen's interest into this direction. In addition, he joined forces with Lutek Wolniewicz from the Nicolaus Copernicus University, Toruń, Poland, to explore the usefulness of hyperspherical coordinates and hyperspherical functions as tools to describe the quantum dynamics in three-particle systems. A first study, using hyperspherical coordinates for a quantum mechanical description of the three-dimensional reactive scattering process, was made in the thesis of Heinrich Wippermann (1989). The method development continued in collaboration with Lutek Wolniewicz and Alexander Alijah. Quite naturally, the protonated hydrogen molecule, H_3^+, and its isotopomers were the first systems to which the new method was applied, with great success. Aspects of symmetry breaking were considered in the thesis of Oliver Friedrich (2000); a complete determination and identification of the rovibrational states of H_3^+, up to about 13,000 cm^{-1} above its ground state, was achieved in the thesis of Peter Schiffels (2002). Further works considered the adiabatic approximation and non-adiabatic effects in three-particle systems. As Takeshi Oka remarked, "Juergen has contributed greatly to the science of H_3^+ at the most fundamental level" with these developments [6]. Juergen was also interested in electron-atom and electron-molecule scattering. With Peter Hamacher, who completed his thesis in 1990, non-relativistic and relativistic versions of program codes for variational *R*-matrix scattering calculations were developed. Fundamental problems of the relativistic *R*-matrix theory were discussed and solved in joint work with Radek Szmytkowski, who came as a postdoc from the group of Eugeniusz Czuchaj at the University of Gdańsk, Poland, and is now Professor at Gdańsk University of Technology.

Many other research topics attracted Juergen's interest. He published papers, e.g., on the theory of reaction dynamics (with his diploma student Klaus-Peter Karmann), on perturbation theory combined with the variation principle (with Jerry Silverman, then at the Department of Chemistry, University of Stirling, Stirling, United Kingdom.), on the local-scaling transformation version of density functional theory (with Eduardo Ludeña from the Instituto Venezolano de Investigaciones Científicas, Caracas, Venezuela, Eugene Kryachko from the Bogolubov Institute of Theoretical Physics, Kiev, Ukraine, and Toshikatsu Koga from the Muroran Institute of Technology, Japan), on extended line notations for coding of chemical formulas and structures (with his coworker Udo Welz and his doctoral student Andreas Bruder), on fundamental

relations between parameters in density functional theory, and on 'non-trivial zeroes' of angular momentum coupling coefficients (with Ravi Rau from the Department of Physics and Astronomy, University of Louisiana, Baton Rouge, Louisiana). The list of publications following this biography provides further details.

Several of Juergen's research contributions were fundamental and later proved to be essential for further developments, though sometimes with quite large time delay. For example, his work on the theory of the MCSCF method from 1973, written with electronic (fermionic) systems in mind, proved to be important about 25 years later for the development of vibrational MCSCF methods [7]. It is worth to mention in this context that according to Juergen's conviction, only the essentials of scientific work should be published. He became more and more concerned about the future of high-quality science, and early on expressed his view on the publication explosion, at least partly caused by what he called the failure of the peer-review system. As partial solutions, he suggested (1) to moderately reimburse the referees for their efforts, and (2) to stop judging scientists and their work merely by simple counting criteria. Imposing a refereeing system based on fees, similar or comparable to consulting practices in other branches (e.g., law, medicine), might work well in the exact sciences if the authors have to carry the charge in case of reject of their article, but if the publisher takes it over in case of acceptance. As to the misapplication of counting criteria, Juergen could have asked, "How could it happen that so many decision makers in what claim to be highly developed countries base their decisions on criteria requiring no higher intellectual skills than those acquired already in the first school years, namely counting numbers, up to several orders of magnitude? How could it happen that counting is self-deceptively taken for measuring?" Do we have forgotten that the quote "Measure what is measurable, and make measurable what is not so", attributed to Galileo Galilei, does not exclude failure, i.e., non-existence of a measure, as a possible correct answer? Under the headline "Quality not Quantity," the *Deutsche Forschungsgemeinschaft* (DFG) announced, early this year, to change a paradigm in research funding [8]: new regulations adopted for funding proposals impose upper limits on the number of own publications scientists are allowed to cite in their proposals. This measure, taken to counter the flood of publications in research, follows similar regulations now imposed by the NSF and the NIH. Presumably, Juergen might have called this a step in the right direction.

Juergen has been a member of several national and international scientific societies, including the *Gesellschaft Deutscher Chemiker* (GDCh), the *Deutsche Physikalische Gesellschaft* (DPG), the *Deutsche Bunsen-Gesellschaft für Physikalische Chemie*, the European Physical Society (EPS), the American Chemical Society (ACS), the American Physical Society (APS), and the American Geographical Society. He acted as a member of the editorial board of the *Lecture Notes in Chemistry* series of monographs from 1984 until discontinuation of the series in 2004. At Bielefeld, he was chairman of the local chapter of the GDCh from 1975, the year of his appointment, till 1996. He also served as chairman of the chemistry department in the years 1977–1979 and 1989–1990 and was a member of the university's senate from 1979 to 1991.

Science was not Juergen's sole affection, he also liked to play tennis, to go for skiing, and he was a passionate yachtsman. A trophy received for a first place in the Flying Dutchman class, in a regatta on Lake Michigan in 1970, always decorated his office desk. Cruising with a sail boat along some distant coasts was one of his favorite summer activities. He has also been an enthusiastic chef-de-cuisine, and guests invited to his home may recollect delicious meals enjoyed with witty conversations. Since his sudden and unexpected death, on October 10, 2008 in Bielefeld, such recollections are to be treasured.

References

1. Liu B (1973) J Chem Phys 58:1925
2. Saxon R (1999) Mol Phys 96:465
3. Schaefer III HF (1984) Quantum Chemistry. Clarendon, Oxford
4. Steimle TC et al (1986) J Chem Phys 85:1276
5. Bishop DM (1999) In: Maksić ZB, Orville-Thomas WJ (eds) Pauling's legacy: modern modelling of the chemical bond. Elsevier, Amsterdam, p 129
6. Oka T (2008) Private communication (Oct 14)
7. Drukker K, Hammes-Schiffer S (1997) J Chem Phys 107:363
8. DFG, press release no. 7. 23 Feb 2010. Available via http://www.dfg.de/en/service/press/press_releases/index.html

Publication list and other bibliographic data

"*One can measure the importance of a scientific work by the number of earlier publications rendered superfluous by it*."

David Hilbert (1862–1943, German mathematician)

Titles in German are supplemented by translations to English.

Edited books

1. D. A. Ramsay and J. Hinze (eds.): *Selected Papers of Robert S. Mulliken*, University of Chicago Press, Chicago, 1975 (XIV, 1127 pp.).
2. J. Hinze (ed.): *The Permutation Group in Physics and Chemistry* (Lecture Notes in Chemistry Vol. 12), Springer, Berlin, 1979 (VI, 230 pp.).
3. J. Hinze (ed.): *The Unitary Group for the Evaluation of Electronic Energy Matrix Elements* (Lecture Notes in Chemistry Vol. 22), Springer, Berlin, 1981 (VI, 371 pp.).
4. J. Hinze (ed.): *Numerical Integration of Differential Equations and Large Linear Systems* (Lecture Notes in Mathematics Vol. 968), Springer, Berlin, 1982 (VI, 412 pp.).
5. J. Hinze (ed.): *Electron-Atom and Electron-Molecule Collisions*, Plenum, New York, 1983 (VIII, 354 pp.).
6. J. Hinze (ed.): *Energy Storage and Redistribution in Molecules*, Plenum, New York, 1983 (XI, 615 pp.).

Scientific papers and PhD thesis

1. J. Hinze and H. H. Jaffé: Electronegativity. I. Orbital Electronegativity of Neutral Atoms. *J. Am. Chem. Soc*. 84: 540–546, 1962.
2. Jürgen A. Hinze: *Electronegativity*. PhD thesis, University of Cincinnati, 1962 (311 pp.).
3. J. Hinze, M. A. Whitehead and H. H. Jaffé: Electronegativity. II. Bond and Orbital Electronegativities. *J. Am. Chem. Soc*. 85: 148–154, 1963.
4. J. Hinze and H. H. Jaffé: Electronegativity. III. Orbital Electronegativities and Electron Affinities of Transition Metals. *Can. J. Chem*. 41: 1315–1328, 1963.
5. J. Hinze and H. H. Jaffé: Electronegativity. IV. Orbital Electronegativities of the Neutral Atoms of the Periods Three A and Four A and of Positive Ions of Periods One and Two. *J. Phys. Chem*. 67: 1501–1506, 1963.
6. J. Hinze and H. H. Jaffé: Slater-Condon Parameters from Spectral Data. *J. Chem. Phys*. 38: 1834–1847, 1963.
7. J. Hinze and K. S. Pitzer: Ionic or *d*-Hybrid Bonds in Noble-Gas Halides. In H. Hyman (ed.): *Noble-Gas Compounds*, University of Chicago Press, Chicago, 1963, pp. 340–346.
8. J. Hinze and K. S. Pitzer: Atomic Integrals Containing Functions of r_{12} and r_{13}. *J. Chem. Phys*. 41: 3484–3487, 1964.
9. J. Hinze and R. F. Curl, Jr.: Infrared Spectrum of N-Methylenemethylamine. *J. Am. Chem. Soc*. 86: 5068–5070, 1964.
10. J. T. Yardley, J. Hinze and R. F. Curl, Jr.: Equilibrium Conformation of *N*-Methylenemethylamine from Microwave Data. *J. Chem. Phys*. 41: 2562–2563, 1964.
11. C. F. Chang, B. J. Fairless, M. R. Willcott, R. F. Curl, Jr., J. Hinze, D. F. Koster and A. Danti: Proton Magnetic Resonance Spectrum and Nuclear Overhauser Effects of *N*-Methylmethylenimine. *J. Mol. Spectrosc*. 22: 112–117, 1967.
12. J. Hinze and C. C. J. Roothaan: Multi-Configuration Self-Consistent-Field Theory. *Suppl. Prog. Theor. Phys*. 40: 37–51, 1967.
13. J. Hinze: Elektronegativität der Valenzzustände (Electronegativity of valence states). *Fortschr. Chem. Forsch*. 9: 447–485, 1968 (in German).
14. N. Sabelli and J. Hinze: Atomic Multiconfiguration Self-Consistent Field Wavefunctions. *J. Chem. Phys*. 50: 684–700, 1969.
15. J. Hinze: Optimization of Exponents for Slater-Type Basis Functions. *J. Chem. Phys*. 51: 4168–4169, 1969.
16. J. Hinze: Heteropolar Bonds. In H. Eyring, D. Henderson and W. Jost (eds.): *Valency* (Physical Chemistry, Vol. V), Academic Press, New York, 1970, pp. 173–204.
17. D. L. Beveridge and J. Hinze: Parametrization of Semi-Empirical π-Electron Molecular Orbital Calculations. π-Systems Containing Carbon, Nitrogen, Oxygen and Fluorine. *J. Am. Chem. Soc*. 93: 3107–3114, 1971.
18. G. C. Lie, J. Hinze and B. Liu: Calculated $a^4\Sigma^-$, $A^2\Delta$, $B^2\Sigma^-$ States of CH. *J. Chem. Phys*. 57: 625–631, 1972.
19. K. K. Docken and J. Hinze: LiH Potential Curves and Wave Functions for $X^1\Sigma^+$, $A^1\Sigma^+$, $B^1\Pi$, $^3\Sigma^+$ and $^3\Pi$. *J. Chem. Phys*. 57: 4928–4936, 1972.
20. K. K. Docken and J. Hinze: LiH Properties, Rotation-Vibrational Analysis and Transition Moments for $X^1\Sigma^+$, $A^1\Sigma^+$, $B^1\Pi$, $^3\Sigma^+$ and $^3\Pi$. *J. Chem. Phys*. 57: 4936–4952, 1972.
21. J. Hinze: Large CI versus MC-SCF. In D. W. Smith and W. B. McKae (eds.): *Energy, Structure and Reactivity*, Wiley, New York, 1973, pp. 170–178.
22. G. C. Lie, J. Hinze and B. Liu: Valence Excited States of CH. I. Potential Curves. *J. Chem. Phys*. 59: 1872–1886, 1973.

23. G. C. Lie, J. Hinze and B. Liu: Valence Excited States of CH. II. Properties. *J. Chem. Phys*. 59: 1887–1898, 1973.
24. J. Hinze: MC-SCF. I. The Multi-Configuration Self-Consistent-Field Method. *J. Chem. Phys*. 59: 6424–6432, 1973.
25. J. Hinze: An Overview of Computational Methods for Large Molecules. *Adv. Chem. Phys*. 26: 213–263, 1974.
26. W. M. Kosman and J. Hinze: Accuracy in Determining the Potential Energy Curve Minimum. *J. Mol. Spectrosc*. 51: 341–350, 1974.
27. C. W. Eaker and J. Hinze: Semiempirical MC-SCF Theory. I. Closed Shell Ground State Molecules. *J. Am. Chem. Soc*. 96: 4084–4089, 1974.
28. J. Hinze, R. Solarz and D. H. Levy: A Mechanism for the Production of Unequal Bond Lengths in Some States of AB_2 Triatomic Molecules. *Chem. Phys. Lett*. 25: 284–286, 1974.
29. J. Hinze, G. C. Lie and B. Liu: Valence Excited States of CH. III. Radiative Lifetimes. *Astrophys. J*. 196: 621–631, 1975.
30. E. S. Sachs, J. Hinze and N. H. Sabelli: MCSCF Calculations for Six States of NaH. *J. Chem. Phys*. 62: 3367–3376, 1975.
31. E. S. Sachs, J. Hinze and N. H. Sabelli: Rotation-Vibrational Analysis for Three States of NaH and NaD. *J. Chem. Phys*. 62: 3377–3383, 1975.
32. E. S. Sachs, J. Hinze and N. H. Sabelli: Transition Moments, Band Strengths and Line Strengths for NaH. *J. Chem. Phys*. 62: 3384–3388, 1975.
33. E. S. Sachs, J. Hinze and N. H. Sabelli: Calculation of the Far-Wing Line Broadening of the Sodium *D* Line Induced by Collisions with Hydrogen Atoms. *J. Chem. Phys*. 62: 3389–3392, 1975.
34. E. S. Sachs, J. Hinze and N. H. Sabelli: Frozen Core Approximation, a Pseudopotential Method Tested on Six States of NaH. *J. Chem. Phys*. 62: 3393–3398, 1975.
35. W. M. Kosman and J. Hinze: Inverse Perturbation Analysis: Improving the Accuracy of Potential Energy Curves. *J. Mol. Spectrosc*. 56: 93–103, 1975.
36. F. L. Tobin and J. Hinze: The Eigenvalue Problem for a Double Minimum Potential. *J. Chem. Phys*. 63: 1034–1035, 1975.
37. D. H. Levy and J. Hinze: Hyperfine and Λ-Doubling Splitting in Excited Rotational Levels of CH. *Astrophys. J*. 200: 236–238, 1975.
38. C. W. Eaker and J. Hinze: Decomposition of 1,2-Dioxetane. *Theor. Chim. Acta* 40: 113–118, 1975.
39. D. H. Levy and J. Hinze: The Predicted Λ-Doubling Spectrum of ^{13}CH. *Astrophys. J*. 211: 980–984, 1977.
40. L. Engelbrecht and J. Hinze: Computer Determination of Molecular Properties for Diatomics. In E. V. Ludeña, N. H. Sabelli and A. C. Wahl (eds.): *Computers in Chemical Education and Research*, Plenum, New York, 1977, pp. 309–336.
41. E. Yurtsever and J. Hinze: Cusp Conditions with Gauss Type Basis Functions. *J. Chem. Phys*. 69: 3431–3432, 1978.
42. A. Golebiewski, J. Hinze and E. Yurtsever: The Orthogonal Gradient Method. A Simple Method to Solve the Closed-Shell, Open-Shell, and Multiconfiguration SCF Equations. *J. Chem. Phys*. 70: 1101–1106, 1979.
43. T. Voegel, J. Hinze and F. Tobin: Numerical SCF Method for the Calculation of Static Polarizabilities and Hyperpolarizabilities for Atoms, He through Ne. *J. Chem. Phys*. 70: 1107–1111, 1979.
44. F. Tobin and J. Hinze: Numerical MCSCF Methods for Molecules. I. Theory of Unicenter Expansions. *J. Chem. Phys*. 70: 1751–1758, 1979.
45. J. Hinze and E. Yurtsever: An Algorithm to Solve Open- and Closed-Shell and Restricted MC-SCF Equations. *J. Chem. Phys*. 70: 3188–3190, 1979.
46. E. Yurtsever and J. Hinze: The Hellmann-Feynman Theorem for Open-Shell and Multiconfiguration SCF Wave Functions. *J. Chem. Phys*. 71: 1511, 1979.
47. K.-P. Karmann and J. Hinze: Multiple Stationary Points in Open Chemically Reacting Systems. Minimal Requirements. *J. Chem. Phys*. 72: 5476–5478, 1980.
48. L. Engelbrecht and J. Hinze: Molecular Properties Observed and Computed. *Adv. Chem. Phys*. 44: 1–141, 1980.
49. J. Hinze: Large Eigenvalue Problems in Quantum Chemistry. In J. Hinze (ed.): *Numerical Integration of Differential Equations and Large Linear Systems* (Lecture Notes in Mathematics Vol. 968), Springer, Berlin, 1982, pp. 361–369.
50. J. Hinze and A. Golebiewski: MCSCF Using the Generalized Fock Operator. In *Recent Developments and Applications of Multi-Configuration Hartree-Fock Methods* (NRCC Proceedings No. 10, LBL-12157, UC-4, CONF-800726), National Resource for Computation in Chemistry, 1981, pp. 1–9.
51. J. Hinze and J. T. Broad: CI-Energy Expressions in Terms of the Reduced Density Matrix Elements of a General Reference. In J. Hinze (ed.): *The Unitary Group for the Evaluation of Electronic Energy Matrix Elements* (Lecture Notes in Chemistry Vol. 22), Springer, Berlin, 1981, pp. 332–344.
52. J. Hinze: Developments in the Calculation of Electronic Wave functions for Molecules: MCSCF, CI

and Numerical SCF for Molecules. *Int. J. Quantum Chem., Quantum Chem. Symp*. 15: 69–90, 1981.
53. J. Hinze: Operator Methods for MCSCF. In *CCP1 News-letter*, Daresbury Laboratory, 1981.
54. J. Hinze: New Developments in the MCSCF Method. In R. Carbó (ed.): *Current Aspects in Quantum Chemistry 1981* (Studies in Physical and Theoretical Chemistry, Vol. 21), Elsevier, Amsterdam, 1982, pp. 167–179.
55. J. Hinze: Jahresrückblick: Theoretische Chemie 81 (Annual Review: Theoretical Chemistry 81). *Nachr. Chem. Techn. Lab*. 30: 126–131, 1982 (in German).
56. J. Hinze: Elektronegativität: Relikt oder Renaissance? (Electronegativity: relic or renaissance?) *Chimia* 36: 465–466, 1982 (in German).
57. J. Hinze: Jahresrückblick: Theoretische Chemie 82 (Annual Review: Theoretical Chemistry 82). *Nachr. Chem. Techn. Lab*. 31: 111–114, 1983 (in German).
58. K. V. Dinesha and J. Hinze: Configuration Interaction Matrix Elements for Atoms Using Permutation Group Algebra. *Int. J. Quantum Chem*. 26: 507–519, 1984.
59. J. Hinze: Jahresrückblick: Theoretische Chemie 83 (Annual Review: Theoretical Chemistry 83). *Nachr. Chem. Techn. Lab*. 32: 134–136, 1984 (in German).
60. J. T. Broad and J. Hinze: Calculation of Free-Free Radial Dipole Transition Amplitudes: An L^2 Basis Approach. In H. Kleinpoppen, J. S. Briggs, and H. O. Lutz (eds.): *Fundamental Processes in Atomic Collision Physics* (NATO ASI Series, Ser. B, Vol. 134), Plenum, New York, 1985, pp. 671–676.
61. A. Alijah, J. T. Broad and J. Hinze: Stark Effect and Field Ionization of Atomic Hydrogen. *J. Phys*. B 19: 2617–2627, 1986.
62. L. Wolniewicz and J. Hinze: Atom-Diatomic Molecular Reactive Scattering: Investigation of the Hyperangular Integration. *J. Chem. Phys*. 85: 2012–2018, 1986.
63. F. Biegler-König and J. Hinze: Nonrelativistic Numerical MCSCF for Atoms. *J. Comput. Phys*. 67: 290–309, 1986.
64. J. N. Silverman and J. Hinze: High-Order Stark Effect Perturbation Series for Hydrogenic Ions via the Perturbational-Variational Rayleigh-Ritz Formalism. *Chem. Phys. Lett*. 128: 466–473, 1986.
65. D. Bergmann and J. Hinze: Electronegativity and Charge Distribution. *Struct. Bonding (Berlin)* 66: 145–190, 1987.
66. J. N. Silverman and J. Hinze: Calculation of High-Order Electric Polarizabilities via the Perturbational-Variational Rayleigh-Ritz Formalism: Application to the Hydrogenic Stark Effect. *Phys. Rev*. A 37: 1208–1222, 1988.
67. P. Hamacher and J. Hinze: The Variational *R*-Matrix Method: Resonances in the Photoionisation of He for Photon Energies 58–65 eV. *J. Phys*. B 22: 3397–3410, 1989.
68. A. Alijah, J. Hinze, and J. T. Broad: Photoionisation of Hydrogen in a Strong Magnetic Field. *J. Phys*. B 23: 45–60, 1990.
69. J. Hinze and P. Hamacher: Variation Determination of Optimal Orbitals for Electron Scattering. *J. Chem. Phys*. 92: 4372–4373, 1990.
70. J. Hinze and F. Biegler-König: Numerical Relativistic and Non-Relativistic MCSCF for Atoms and Molecules. In R. Carbó and M. Klobukowski (eds.): *Self-consistent Fields: Theory and Applications* (Studies in Physical and Theoretical Chemistry, Vol. 70), Elsevier, Amsterdam, 1990, pp. 405–446.
71. J. Hinze. Wissenschaftliche Bibliothek als Informationsspeicher? Als Informationsdienst! (The scientific library as information reservoir? As information service!) *Mitteilungsblatt Verband der Bibliotheken des Landes NRW*, 40(1): 15–17, 1990 (in German).
72. P. Hamacher and J. Hinze: Finite-Volume Variational Method for the Dirac Equation. *Phys. Rev*. A 44: 1705–1711, 1991.
73. L. Wolniewicz, J. Hinze and A. Alijah: Reactive Collisions of Atoms with Diatomic Molecules. *J. Chem. Phys*. 99: 2695–2707, 1993.
74. L. Wolniewicz and J. Hinze: Rotation-Vibrational States of H_3^+ Computed Using Hyperspherical Coordinates and Harmonics. *J. Chem. Phys*. 101: 9817–9829, 1994.
75. M. Rosenberger and J. Hinze: Influence of the Radiation Field onto the Photodissociation. *Chem. Phys*. 189: 41–52, 1994.
76. J. Hinze: Comment on "The Electron Density and Chemical Bonding: A Reinvestigation of Berlin's Theorem" [J. Chem. Phys. 94, 2977 (1991)]. *J. Chem. Phys*. 101: 6369–6370, 1994.
77. A. Alijah, J. Hinze and L. Wolniewicz: Rotation-Vibrational States of H_3^+ Using Hyperspherical Coordinates and Harmonics. *Ber. Bunsen-Ges. Phys. Chem*. 99: 251–253, 1995.
78. J. Hinze, A. Alijah and L. Wolniewicz: Three Particle Systems and Hyperspherical Harmonics. In E. Yurtsever (ed.): *Frontiers of Chemical Dynamics* (NATO ASI Series, Ser. C, Vol. 470), Kluwer, Amsterdam, 1995, pp. 357–369.
79. E. V. Ludeña, E. S. Kryachko, T. Koga, R. López-Boada, J. Hinze, J. Maldonado and E. Valderrama: The Local-Scaling Version of Density-Functional Theory: A Practical Method for Rigorous Calculations in Density Functional Theory. In J. M. Seminario and P. Politzer (eds.): *Modern Density*

Functional Theory: A Tool for Chemistry (Theoretical and Computational Chemistry, Vol. 2), Elsevier, Amsterdam, 1995, pp. 75–124.

80. E. V. Ludeña, R. López-Boada, J. E. Maldonado, E. Valderrama, E. S. Kryachko, T. Koga and J. Hinze: Local-Scaling Transformation Version of Density Functional Theory. *Int. J. Quantum Chem*. 56: 285–301, 1995.
81. J. Stiehler and J. Hinze: Calculation of Static Polarizabilities and Hyperpolarizabilities for the Atoms He through Kr with a Numerical RHF Method. *J. Phys*. B 28: 4055–4071, 1995.
82. A. Alijah, J. Hinze and L. Wolniewicz: Rotation-Vibrational States of H_2D^+ Using Hyperspherical Coordinates and Harmonics. *Mol. Phys*. 85: 1105–1123, 1995.
83. A. Alijah, L. Wolniewicz and J. Hinze: Rotation-Vibrational States of D_3^+ Computed Using Hyperspherical Harmonics. *Mol. Phys*. 85: 1125–1150, 1995.
84. D. Bergmann and J. Hinze: Elektronegativität und Moleküleigenschaften *Angew. Chem*. 108: 162–176, 849(E), 1996; Electronegativity and Molecular Properties. *Angew. Chem., Int. Ed. Engl*. 35: 150–163, 781(E), 1996.
85. R. Szmytkowski and J. Hinze: Convergence of the Non-Relativistic and Relativistic *R*-Matrix Expansions at the Reaction Volume Boundary. *J. Phys*. B 29: 761–777, 3800–3801(E), 1996.
86. R. Szmytkowski and J. Hinze: Kapur-Peierls and Wigner *R*-Matrix Theories for the Dirac Equation. *J. Phys*. A 29: 6125–6141, 1996.
87. J. Hinze and U. Welz: Broad Smiles. In J. Gasteiger (ed.): *Software-Development in Chemistry, Vol. 10*, Springer, Berlin, 1996, pp. 59–65.
88. J. Hinze, F. Biegler-König and A. G. Löwe: Molecular Charge Density Analysis. *Can. J. Chem*. 74: 1049–1053, 1996.
89. D. Andrae and J. Hinze: Numerical Electronic Structure Calculations for Atoms. I. Generalized Variable Transformation and Nonrelativistic Calculations. *Int. J. Quantum Chem*. 63: 65–91, 1997.
90. E. Valderrama, E. V. Ludeña and J. Hinze: Analysis of Dynamical and Nondynamical Components of Electron Correlation Energy by Means of Local-Scaling Density-Functional Theory. *J. Chem. Phys*. 106: 9227–9235, 1997.
91. J. Hinze, A. Alijah and L. Wolniewicz: Understanding the Adiabatic Approximation; The Accurate Data of H_2 Transferred to H_3^+. *Pol. J. Chem*. 72: 1293–1303, 1998.
92. J. Hinze: The Concept of Electronegativity of Atoms in Molecules. In Z. B. Maksić and W. J. Orville-Thomas (eds.): *Pauling's Legacy: Modern Modelling of the Chemical Bond* (Theoretical and Computational Chemistry, Vol. 6), Elsevier, Amsterdam, 1999, pp. 189–212.
93. J. Hinze, O. Friedrich and A. Sundermann: A Study of Some Unusual Hydrides: BeH_2, BeH_2^+, and SH_6. *Mol. Phys*. 96: 711–718, 1999.
94. E. Valderrama, E. V. Ludeña and J. Hinze: Assessment of the Dynamical and Nondynamical Correlation Energy Components for the Beryllium-atom Isoelectronic Sequence. *J. Chem. Phys*. 110: 2343–2353, 1999.
95. E. V. Ludeña, R. López-Boada, V. Karasiev, R. Pino, E. Valderrama, J. Maldonado, R. Colle and J. Hinze: Recent Developments in the Local Scaling Transformation Version of Density Functional Theory. *Adv. Quantum Chem*. 33: 49–70, 1998.
96. M. Reiher and J. Hinze: Self-consistent Treatment of the Frequency-independent Breit Interaction in Dirac-Fock and MCSCF Calculations of Atomic Structures: I. Theoretical Considerations. *J. Phys*. B 32: 5489–5505, 1999.
97. W. H. E. Schwarz, D. Andrae, S. R. Arnold, J. Heidberg, H. Hellmann Jr., J. Hinze, A. Karachalios, M. A. Kovner, P. C. Schmidt and L. Zülicke: Hans G. A. Hellmann (1903–1938). I. Ein Pionier der Quantenchemie (A pioneer of quantum chemistry). *Bunsen-Magazin* 1(1): 10–21, 1999 (in German).
98. W. H. E. Schwarz, A. Karachalios, S. R. Arnold, L. Zülicke, P. C. Schmidt, M. A. Kovner, J. Hinze, H. Hellmann Jr., J. Heidberg and D. Andrae: Hans G. A. Hellmann (1903–1938). II. Ein deutscher Pionier der Quantenchemie in Moskau (A German pioneer of quantum chemistry in Moscow). *Bunsen-Magazin* 1(2): 60–70, 1999 (in German).
99. D. Andrae, M. Reiher and J. Hinze: Numerical Electronic Structure Calculations for Atoms. II. Generalized Variable Transformation in Relativistic Calculations. *Int. J. Quantum Chem*. 76: 473–499, 2000.
100. D. Andrae, M. Reiher and J. Hinze: A Comparative Study of Finite Nucleus Models for Low-lying States of Few-electron High-*Z* Atoms. *Chem. Phys. Lett*. 320: 457–468, 2000.
101. A. R. P. Rau and J. Hinze: Relations Between Parameters of Density Functional Theories Through Exactly Solvable Many-fermion Models. *J. Chem. Phys*. 114: 9754–9757, 2001.
102. D. Andrae, R. Brodbeck and J. Hinze: Examination of Several Density Functionals in Numerical Kohn-Sham Calculations for Atoms. *Int. J. Quantum Chem*. 82: 227–241, 2001.
103. J. Neugebauer, M. Reiher and J. Hinze: Analysis of the asymptotic and short-range behavior of

quasilocal Hartree–Fock and Dirac–Fock–Coulomb electron–electron interaction potentials. *Phys. Rev.* A 65: 032518/1–10, 2002.
104. J. Neugebauer, M. Reiher and J. Hinze: Analytical local electron electron interaction model potentials for atoms. *Phys. Rev.* A 66: 022717/1–11, 059903(E), 2002.
105. P. Schiffels, A. Alijah and J. Hinze: Rovibrational states of H_3^+. Part 1. The Energy Region Below 9000 cm^{-1} and Modelling of the Non-adiabatic Effects. *Mol. Phys.* 101: 175–188, 2003.
106. P. Schiffels, A. Alijah and J. Hinze: Rovibrational states of H_3^+. Part 2. The Energy Region Between 9000 cm^{-1} and 13000 cm^{-1} Including Empirical Corrections for the Non-adiabatic Effects. *Mol. Phys.* 101: 189–209, 2003.
107. M. Reiher and J. Hinze: Four-Component Ab Initio Methods for Atoms, Molecules, and Solids. In B. A. Hess (ed.): *Relativistic Effects in Heavy Element Chemistry and Physics*, Wiley, Chichester, 2003, pp. 61–88.
108. J. Hinze: Publish or Perish—Peer Review. *Nachr. Chem.* 52: 1171, 2004.
109. A. Alijah and J. Hinze: Rotation-vibrational states of H_3^+ and the adiabatic approximation. *Philos. Trans. R. Soc. London* A 364: 2877–2888, 2006.
110. T. A. Heim, J. Hinze and A. R. P. Rau. Some classes of 'nontrivial zeroes' of angular momentum addition coefficients. *J. Phys.* A 42: 175203/1–11, 2009.
111. A. Alijah, D. Andrae and J. Hinze: An empirical formula to estimate off-diagonal adiabatic corrections to rotation-vibrational energy levels. *Theor. Chem. Acc.*, this issue.

Supervised PhD and doctoral theses (in approximate chronological order)

- At the University of Chicago:

1. Bowen Liu: *A Theoretical Study of Three-Electron Systems: He_2^+ and* H_3. 1971 (1975, co-supervised with A. D. McLean, IBM Research Laboratory, San Jose, California).
2. Kate Kirby Docken: *Accurate Ab Initio Calculations of Energy and Properties for Ground and Excited States of Lithium Hydride*. 1972 (169 pp.).
3. George C. Lie: *Valence Excited States of Carbon Hydride*. 1972 (196 pp.).
4. Warren M. Kosman: *Diatomic Potentials; Transcorrelated Wavefunctions: Two Theoretical Studies*. 1974 (51 pp.).
5. Charles W. Eaker: *A Semiempirical MC-SCF Theory*. 1974 (79 pp.).
6. Edward S. Sachs: *Valence Excited States of NaH: A Theoretical Study*. 1975.
7. Frank L. Tobin: *A Feasibility Study for a Numerical Hartree-Fock Method for Molecules*. 1976 (152 pp.).

- At the University of Bielefeld:

8. Thomas Vögel: *Numerisches Hartree-Fock für Moleküle (Numerical Hartree-Fock method for molecules)*. 1981 (75 pp., in German).
9. Alexander Alijah: *Photoionisation des Wasserstoffatoms im starken Magnetfeld (Photoionization of the hydrogen atom in a strong magnetic field)*. 1988 (107 pp., in German).
10. Heinrich K. F. Wippermann: *Quantenmechanische Behandlung des dreidimensionalen reaktiven Streuprozesses in hypersphärischen Koordinaten (Quantum mechanical treatment of the threedimensional reactive scattering process in hyperspherical coordinates)*. 1989 (155 pp., in German).
11. Peter Hamacher: *Die R-Matrix-Eigenwert-Theorie. Resonanzen bei der Elektron-Atom-Streuung und der Photoionisation von Atomen (The R-matrix eigenvalue theory. Resonances in electron-atom scattering and photoionization of atoms)*. 1990 (158 pp., in German).
12. Dieter Bergmann: *Ansätze zur Datenreduktion unter dem besonderen Aspekt von Kraftfeldparametrisierungen (Approaches to data reduction under the particular aspect of force field parameterizations)*. 1992 (230 pp., in German).
13. Hans-Dieter Krumme: *Relativistisches Closed-Shell-Hartree-Fock für 2-atomige Moleküle (Relativistic closed-shell Hartree-Fock method for diatomic molecules)*. 1992 (93 pp., in German).
14. Johannes Stiehler: *Der numerische Multikonfiguration Self-Consistent Field Ansatz für Atome (The numerical multiconfiguration self-consistent field ansatz for atoms)*. 1995 (147 pp., in German), URL: http://bieson.ub.uni-bielefeld.de/volltexte/2009/1516/.
15. Martina Rosenberger: *Zeitabhängige Formulierung des Mehr-Elektronen-Problems in Atomen (Time-dependent formulation of the many-electron problem in atoms)*. 1997 (145 pp., in German), URL: http://bieson.ub.uni-bielefeld.de/volltexte/2009/1519/.
16. Markus Reiher: *Development and Implementation of Numerical Algorithms for the Solution of Multi-Configuration Self-Consistent Field*

Equations for Relativistic Atomic Structure Calculations. 1998 (190 pp.).
17. Oliver Friedrich: *Symmetriebrechung bei kleinen Molekülen (Symmetry breaking in small molecules)*. 2000 (208 pp., in German).
18. Peter Schiffels: *Quantum Dynamics of Triatomic Molecules: A Hyperspherical Description*. 2002 (180 pp.), URL: http://bieson.ub.uni-bielefeld.de/volltexte/2003/224/.
19. Andreas Bruder: *SMILES-3D: das weiterentwickelte Konzept zur Codierung dreidimensionaler Molekülstruktur in einer linearen Notation und die programmtechnische Umsetzung in der Software WinSmiles-3D (SMILES-3D: the advanced concept for coding threedimensional molecular structure with a line notation and its implementation in the software WinSmiles-3D)*. 2003 (192 pp., in German), URL: http://bieson.ub.uni-bielefeld.de/volltexte/2004/503/.
20. Christian Oldiges: *Molecular Dynamics Simulation on Structure-Dynamic Actions in Aqueous Acetonitrile/crosslinked Polyacrylamide Mixtures*. 2003 (104 pp.).
21. Thorsten Tönsing: *Aufbau eines klassenbasierten Programmpaketes zur molekulardynamischen Simulation von Gelen am Beispiel des N-Isopropylacrylamid Hydrogels (Setup of a class-based program package for molecular dynamics simulations of gels using the N-isopropylacrylamide hydrogel as an example)*. 2004 (186 pp., in German), URL: http://bieson.ub.uni-bielefeld.de/volltexte/2004/562/.

Habilitation theses conducted under his mentorship (in chronological order, all at the University of Bielefeld)

1. Wolfgang W. Schoeller: *MO-Modelle in der Organischen Chemie (MO models in organic chemistry)*. 1977 (166 pp., in German).
2. John T. Broad: *Scattering Theory in Special L^2 Bases*. 1984 (142 pp.).
3. Peter Pfeifer: *Fraktale Strukturen in der Chemie (Fractal structures in chemistry)*. 1986 (in German).
4. Alexander Alijah: *Dynamik und Spektren dreiatomiger Moleküle unter Berücksichtigung der starken Kopplung zwischen Rotation, Schwingung und elektronischer Bewegung (Dynamics and spectra of triatomic molecules with consideration of the strong coupling between rotation, vibration and electronic motion)*. 1996 (268 pp., in German).
5. Dirk Andrae: *Entwicklung basissatzfreier Methoden für quantenchemische Rechnungen (Development of basis-set-free methods for quantum chemical calculations)*. 2000 (311 pp., in German).