

## Curriculum Vitae

Ludwik Adamowicz

Born in Warsaw, Poland, January 29, 1950. U.S. Citizen (1991) (Married, four children).

### **Education:** MS, Warsaw University

MS thesis "Mulliken Population Analysis of Water Complexes with Li<sup>+</sup>, Na<sup>+</sup>, F<sup>-</sup> and Cl<sup>-</sup>", 1973, Advisor Professor W. Kolos.

Ph.D., Institute of Physical Chemistry of the Polish Academy of Sciences.

Ph.D. Thesis "Gaussian Geminals Used to Calculate Electronic Correction Energy of Small Molecules", 1977, Advisor Professor A.J. Sadlej.

### **Employment:**

Aug. 1998-present: Professor of Chemistry, University of Arizona. (Primary appointment)

June 2003-present: Professor of Physics, University of Arizona

Feb. 2004- July 2004: Visiting Professor, University of Pisa, Italy

Dec. 2001-Aug. 2002: Visiting Professor, Laboratoire de Physique Quantique, Universite Paul Sabatier, Toulouse, France.

Aug. 2001-Dec. 2001: Visiting Professor, Nagoya University and The Institute for Molecular Science, Okazaki, Japan.

2-1995-8-1995: Visiting Researcher, Laboratoire de Physique Quantique, Universite Paul Sabatier, Toulouse, France. (Sabbatical leave from The University of Arizona)

8-1994-2-1995: Visiting Professor, University of Lund, Lund, Sweden. (Sabbatical leave from The University of Arizona)

1993-1998: Associate Professor of Chemistry (with tenure), The University of Arizona.

1987-1993: Assistant Professor of Chemistry, The University of Arizona.

1983-1987: Research Associate (with R. J. Bartlett), Quantum Theory Project, University of Florida.

1980-1983: Research Associate (with E. A. McCullough), Department of Chemistry and Biochemistry, Utah State University.

1978-1980: Research assistant and director of the computer center at the Institute of Physical Chemistry, Polish Academy of Sciences.

1977-1978: Lecturer at University of Kielce, Poland.

1975-1978: Research assistant in Department of Calorimetry at the Institute of Physical Chemistry, Polish Academy of Sciences and graduate student (with A. J. Sadlej) at Institute of Organic Chemistry, Polish Academy of Sciences.

1973-1974: Research Assistant, Department of Chemistry, Warsaw University

### **Teaching:**

681, Special topic class on application of Quantum Mechanics to Chemistry, Spring 2001

680, Quantum Chemistry II - Spring 1989, Spring 1993, Spring 1997, Spring 2000.

580, Quantum Chemistry I - Fall, 1987, Fall 1988, Fall 1989, Fall 1992, Fall 1996, Fall 1997, Fall 1998.

503, Remedial Physical Chemistry - Fall 1999, Fall 2000, Fall 2002, Fall 2003.

481, Physical Chemistry for Biochemistry majors (lectures & discussions) - Spring 1998, Spring 1999.

480A and B, Physical Chemistry (lectures & discussions) - Fall 1990, Fall 1991, Spring 1991, Fall 2002, Fall 2003.

103A, Fundamentals of Chemistry - Fall 1993, Fall 1995, Spring 1996.

## Honors and Awards:

1977	Award of the Secretary of the Polish Academy of Sciences for Outstanding Ph.D. dissertation.
1978	Award of the Secretary of the Polish Academy of Sciences for Research Accomplishments.
1991	Junior Faculty Research Award of the American Cancer Society.
2001	Fulbright Award

## Former Students and Postdocs Holding Academic Positions:

Maurice Cafiero	Assistant Professor	Rhodes College
Pawel Kozlowski	Assistant Professor	University of Louisville
Piotr Piecuch	Professor	Michigan State University
Gill Rohrig	Assistant Professor	San Diego State University
Dayle Smith	Assistant Professor	Whitman College
Zdenek Slanina	Professor	Molecular-Design Engineering Department, Toyohashi University of Technology, Japan.

## Intramural Service:

### Departmental Committees:

Recruiting Committee member - 1987, 1988.  
Computer Committee member - 1987, 1998, 1999, 2000.  
Departmental Seminar Committee member - 1988.  
Departmental Seminar Committee Chairman - 1989.  
Graduate Study Committee member - 1991, 2000, 2002, 2003.  
TA Evaluation Committee member - 1992, 1993, 1994.  
TA Evaluation Committee Chairman - 1995, 1996, 1997, 1998, 1999, 2000, 2001, 2002, 2003.  
Head of the Physical Chemistry Division - 1996, 1997, 1998.  
Departmental P&T Committee Chairman - 1998.

### University Committees:

Computer Hardware Subcommittee of the Academic Computing Advisory Committee.  
University Computer Committee - 1990.  
Grade Appeal Committee - 1992.  
College Representative in Faculty Senate - 1994, 1995, 1996.

## Extramural Service:

Reviewer for *Chemical Reviews*, *Journal of the American Chemical Society*, *Journal of Physical Chemistry*, *Chemical Physics Letters*, *International Journal of Quantum Chemistry*, *Theoretica Chimica Acta*, *Journal of Computational Chemistry* and *Journal of Chemical Physics*.  
Reviewer of proposals submitted to the National Science Foundation, Petroleum Research Fund, National Research Council, and Department of Energy.

### Recent Invited Conference Lectures

- 2004 EURESCO Conference, "Molecules of Biological Interest in the Gas Phase", Exeter, England.
- 2004 European Conference on Molecular Spectroscopy, Krakow, Poland.
- 2004 International Conference on Theoretical Methods of Quantum Chemistry, St. Simons Isl. Georgia.
- 2004 Workshop of New Methods of Quantum Chemistry, Pisa, Italy.

### Grants and Contracts

- 1988 PI, Institutional Cancer Research Grant; one year, \$8,000.
- 1987 PI, NATO travel grant to attend NATO ARW in Versailles, France; \$3,000.
- 1988 PI, Biomedical Research Support Grant; one year, \$8,000.
- 1988 PI, NRC travel grant to attend UPAC Conference in Stockholm, Sweden; \$700.
- 1989 PI, IBM Research Support Grant, \$2,000 + 150 cpu hours on IBM 3090.
- 1989 PI, Grant from International Project Development Fund, University of Arizona for research collaboration with Mexico, \$920; and Poland, \$1,500.
- 1989 Co-PI, NSF; Shared Instrumentation Program; "Mini Supercomputer"; \$500,000.
- 1990 PI, NSF, CHEM-9002748; "Effective Method for Generating Non-Adiabatic Many-Body Wave Function"; two years, \$48,138.
- 1990 Co-PI, NSF; Shared Instrumentation Program; "Mini Supercomputer"; \$115,000.
- 1991 PI, NSF, INT-9016267; "Hydrolysis of Phosphate Esters"; in collaboration with Professor I. Ortega-Blake from UNAM, Cournavaca, MEXICO; three years, \$17,815.
- 1991 PI, NSF; Travel Award to attend Menton Quantum Chemistry Congress; \$1,500.
- 1991 PI, Junior Faculty Research Award of the American Cancer Society, JRF A-334; three years, \$90,500.
- 1991 PI, NSF, INT-9100935; "Theoretical and Experimental Studies on the Spontaneous and Radiation-Induced Tautomerism in Nucleic Acid Bases"; in collaboration with Professor M. Nowak, Institute of Physics, The Polish Academy of Sciences, Warsaw, Poland; three years, \$26,438.
- 1991 PI, Material Characterization Program (MCP); "Theoretical Study on Carbon Vapor"; one year, \$2,100.
- 1992 PI, Material Characterization Program (MCP); "Theoretical Study on Carbon Vapor and Silicon Fibers"; one year, \$1,350.
- 1993 PI, Department of Energy, DEFG0393ER61605; "Theoretical Studies on Radiation-Induced Transformations in Nucleic Acid Bases"; three years, \$290,000.
- 1992 PI, National Research Council; Cooperation in Applied Science and Technology (CAST) program grant to host Dr. Gennady Gutsev from Russia; nine months, \$11,100.
- 1993 PI, NSF, CHE-9300497; "Multi-Reference Coupled Cluster Theory Theoretical Study on Singly- and Doubly-Charged Elemental Cluster Anions"; three years, \$164,700.
- 1993 Co-PI, NSF, Shared Instrumentation Program; "Workstation Cluster for Computational Chemistry"; \$216,000.
- 1993 PI, NATO, CRG931288; "IR and Theoretical Study on Hydrogen Bondings of Nucleic Bases"; in collaboration with Professor G.H. Maes, Katholieke Universit at, Leuven, Belgium; one year, 204,000 Belgian francs.
- 1994 PI, NSF, INT-9313268; "Hydrolysis of Phosphate Esters", Research Group, in collaboration with Professor I. Ortega-Blake from UNAM, Cournavaca, Mexico; three years, \$25,000.
- 1994 Visiting Professor Scholarship of the Natural Sciences Research Council of Sweden; 102,000 Swedish krona.
- 1995 Visiting Researcher Scholarship of CNRS of France; 96,000 French francs.
- 1995 PI, NATO; "IR and Theoretical Study on Hydrogen Bondings of Nucleic Bases", in collaboration with Professor G.H. Maes, Katholieke Universit at, Leuven, Belgium; one year, 235,000 Belgian francs.
- 1996 PI, NATO; "IR and Theoretical Study on Hydrogen Bondings of Nucleic Bases"; in collaboration with

- Professor G.H. Maes, Katholieke Universiteit, Leuven, Belgium; one year, 260,000 Belgian francs.
- 1996 PI, National Research Council, COBAS; to host Dr. Stepan Stepanian from University of Kharkov, Ukraine; six months, \$13,500.
- 1997 PI, NSF, INT-9603373; "Multi-Reference Self-Consistent Size Extensive Configuration Interaction"; in collaboration with Professor J.-P. Malrieu, Paul Sabatier University, Toulouse, France; three years, \$18,000.
- 1998 PI, NSF, CHE-9734821; "Multi-Reference State-Selective Coupled-Cluster Theory"; three years, \$215,000.
- 1998 PI, NSF, CHE-9842766; "Multi-Reference State-Selective Coupled-Cluster Theory", International Supplement to host Dr. V. Ivanov; two years, \$20,080.
- 1998 PI, NATO; "Matrix-Isolation IR and *Ab-Initio* Theoretical Studies of Complexes of DNA Bases"; in collaboration with Dr. Stepan Stepanian, University of Kharkov, Ukraine; two years, 299,000 Belgian francs.
- 1998 PI, Merck Graduate Fellowship for Mrs. Dayle Smith; two years, \$40,000.
- 2000 PI, NSF, CHE-0042603; "Multi-Reference State-Selective Coupled-Cluster Theory"; International Supplement to host Dr. V. Ivanov; one year, \$10,910.
- 2000 PI (with Professor Miguel Duran), Fulbright Foundation and U.S.-Spain Joint Committee for Science and Technology; "Modeling of New Nonlinear Optics Materials with Nonlinearity Enhanced by Proton Transfer"; \$14,800.
- 2000 PI, Sun Microsystems Computer Company, Sun Ultra 10 Model 440 workstation cluster (8 processors), \$29,350.
- 2001 PI, Fulbright award, collaboration project with Laboratoire de Physique Quantique, Universite Paul Sabatier, France
- 2001 PI, Japan Society for the Promotion of Sciences Fellowship, ¥500,000/month for 6 months
- 2001 PI, CNRS-France, Fellowship, 10 months, 22271 ff/month
- 2001 PI, Foreign Travel Grant to attend and present a paper at the Japan Annual Meeting on "Molecular Structure and Spectroscopy" in July, \$500.00.
- 2002 PI, NATO; "Modeling and Testing of New Organic Materials for Light-Emitting Diodes", In collaboration with Dr. Stepan Stepanian, University of Kharkov, Ukraine; two years, 250,000 Belgian francs.
- 2002 PI, DAAD; Study Visit - Theoretical and Computational Chemistry Dusseldorf, Germany, 3892,10 DM/month
- 2003 NSF-(Multi-Investigator Grant), Reversible and Directional Self-Assembly of Bio-Molecular Templates for Nanotechnology Interconnects," \$1,200,000.00.
- 2003 NSF – INT, "Relativistic Molecular Quantum Mechanics Calculations without the Non-Born-Oppenheimer Approximation," collaboration with Dr. Maria Barysz, Torun, Poland, \$32,000.00.
- 2003 NASA – (Multi –Investigator Grant),"Astronomical Search for the Essential Ingredients of Life," \$4,992,929.00.
- 2004 University of Arizona, ISBS Program, DNA Transistor, \$50,000.

### Research Group

#### **Research Associates:**

**Dr. Piotr Piecuch**, now a professor at Michigan State University, joined us for one and a half years in 1991-1993, and worked on theoretical formulation and computational implementation of the fully-exponential SSMRCC scheme and on developing improved methods for converging the CC amplitude equations.

**Dr. Keya Ghose**, after completing her Ph.D. degree with Professor S. Pal in Puna, India, stayed for one year with my group in 1994-1995 and worked on implementation of the recursively calculated intermediates and on the property calculations. She is now back in India and works at the New Delhi University.

**Dr. Zdenek Slanina**, now a professor at the Laboratory of Molecular-Design Engineering, Toyohashi University of Technology, Japan, stayed for one year in my group in 1991-1992 and worked on carbon clusters, fullerenes, and related projects.

**Dr. Genady Gutsev**, currently at Jackson State University, spent two years in my group (first year of his stay was funded by a grant from the CAST program) in 1993-1995, and did calculations on molecular and cluster anions.

**Dr. Don Kinghorn**, worked with my group for four years in 1995-2000 on implementations of explicitly correlated gaussian functions to non-BO atomic and molecular calculations and to the general N-body vibrational

problem and has just completed work on the key integral and gradient formulas for the work presented here. He is now employed by Pulay's computer company in Arkansas.

**Dr. Vladimir Ivanov** worked for a year in my group in 1999-2000 on development and implementation of MRCASCC methodology.

**Dr. Maksym Volobuyev** worked in my group in 2004 on development and implementation of methods for computational simulation of hole transport in DNA.

#### **Graduate Students:**

**Dr. Pawel Kozlowski** received his Ph.D. degree in 1992 and is currently an assistant professor in the Department of Chemistry, University of Louisville, Kentucky. He made a significant contribution to the conceptual framework of the SSM-RCC theory and its implementation; developed the non-BO approach to multi-body systems and implemented explicitly correlated gaussian functions to perform application calculations for those systems.

**Dr. Nevin Oliphant** received his Ph.D. degree in 1991 and is currently with a computer company serving the Wall Street Stock Exchange. He made a significant contribution to the conceptual framework of the SSMRCC theory and its implementation; developed the non-BO approach to multi-body systems and implemented explicitly correlated gaussian functions to perform application calculations for those systems.

**Mr. Z. (John) Zhang** continued Pawel's work on correlated gaussians and implemented analytical derivatives for optimization of the variational wave functions small atoms. He moved to get his Ph.D. degree in analytical chemistry at another university.

**Dr. Yasser Elkadi** completed his Ph.D. degree in 2000 on dipole-bound anionic states of molecules and cluster systems. He is currently employed by Schott-Donnelly Corporation.

**Dr. William McCarthy**, who graduated with a Ph.D. in 1996 and moved to Utah State University to join Professor S. Aust's group, developed methodology for describing large-amplitude vibrations in larger molecular systems.

**Dr. Vadim Alexandrov** who graduated with a Ph.D. in 2001 worked on development of a wave-packet time-propagation method, which he applied to study intra- and inter-molecular proton transfer reactions. Vadim is currently pursuing a second Ph.D. degree in Biophysics at Yale University.

**Mr. Doug Gilmore**, before moving to Law School in Concord, New Hampshire, developed a technique for optimizing multi-center correlated gaussians based on analytical gradients.

**Dr. Dayle Smith** who graduated with a Ph.D. in 2001 studied intra-molecular hydrogen-bonding systems involving DNA bases and electron attachment and transfer in these systems. She is now a Assistant Professor at Whitman College.

**Dr. Mauricio Cafiero** who graduated with a Ph.D. in 2002 worked on implementing explicitly correlated n-electron gaussian functions in Born-Oppenheimer and non-Born-Oppenheimer calculations of molecular systems. He is now an assistant professor at Rhodes College.

**Mr. Sergiy Bubin** joined my group in 2001 and started working on non-Born-Oppenheimer methods for triatomic systems.

**Dr. Michael Nugent** joined my group in 2002 and started his research on the multi-reference coupled cluster method.

#### **Undergraduate Students:**

**Mr. Nathan Oylar**, currently a graduate student at the Department of Chemistry, University of Washington, investigated dipole-bound anionic states of nucleic acid bases.

**Mr. Chris Tarsitano**, currently a graduate student at the University of Chicago, worked on three-body vibrational calculation using the methodology developed in our group.

**Mr. Abraham Jalbout**, currently a student at the University of New Orleans studied chiral selectivity in dipole-electron attachment processes in molecule clusters.

**Ms. Caitlin Hall**, studies excess electron trapping in molecular complexes.

#### **Visiting Scientists:**

**Professor Jong Lee** from Chonbuk National University, South Korea, spent his sabbatical year in my group

working on electronic excitations of chain carbon clusters.

**Dr. Johan Smets**, currently with Proctor and Gamble Corporation in Brussels, visited us twice for three-month periods (his stay was supported by a grant from NATO) and worked on assignment of IR spectra of water complexes of nucleic acid bases based on the theoretically predicted frequencies.

**Dr. Stepan Stepanian** visited us twice for six months in 1997 on a COBASE fellowship and in 1998 using NATO funding and calculated and assigned experimental IR matrix-isolation spectra of pyrimidine-quinone and quinone-quinone dimers and the spectra of some aminoacids and small peptides.

**Ms. Kristien Schoone** and **Ms. Riet Ramaekers** from the University of Leuven visited us for a month in 1997 and worked with our group on the NATO project.

**Ms. Marta Fores**, from the University of Girona, visited for three months and worked on calculations concerning excited-state proton transfer reactions.

**Dr. Humberto Saint-Martin and Prof. Ivan Ortega-Blake**, from UNAM, Mexico, visited my group for two months in the summer 2000 and worked on calculations related to the electron transfer reactions.

**Dr. Josep Maria Louis** from the University of Girona visited my group in August and September 2002 and worked with us on using non-BO methods to calculate electrical properties of small molecules.

**Mr. Bartosz Traskowski** from the University of Warsaw worked in my group in 2004 on projects related to molecular recognition in biological nano-materials.

**Mr. Dariusz Kedziera** from the University of Torun visited my group in the Fall of 2004 and worked on implementation of mass-velocity correction calculations in our non-Boru-Oppenheimer method.

9/27/04